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(54) Title: CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

(57) Abstract: The present invention provides three-dimensional structural information from the hyperthermophilic bacterium Aquifex aeolicus which is a histone deacetylase-like protein (HDLP). HDLP shares 35.2% amino acid sequence identity with human histone deacetylase (HDAC1). The present invention further provides three-dimensional structural information of HDLP bound by inhibitor molecules. The three-dimensional structural information of the present invention is useful to design, isolate and screen deacetylase inhibitor compounds capable of inhibiting HDLP, HDAC family members and HDLP-related molecules. The invention also relates to nucleic acids encoding a mutant HDLP which facilitates the determination of the three-dimensional structure of HDLP in the presence of a zinc atom.



CRYSTAL STRUCTURE OF A DEACETYLASE AND INHIBITORS THEREOF

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This application claims priority of U.S. Provisional Application No. 60/152,753, filed September 8, 1999, the contents of which are hereby incorporated by reference.

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This invention has been made with government support under National Institutes of Health Grant No. RO1 CA-65698. Accordingly, the U.S. Government may have certain rights in the invention.

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Throughout this application, various publications are referenced by author, date and citation. The disclosures of these publications in their entireties are hereby incorporated by reference into this application in order to more fully describe the state of the art as known to those skilled therein as of the date of the invention described and claimed herein.

Introduction

The present invention relates to a histone deacetylase homologue from the hyperthermophilic bacterium Aquifex aeolicus, HDLP (histone deacetylase like protein; also known as AcuCl), which shares 35.2 % sequence identity with human histone deacetylase (HDACl), that can be co-crystallized with an inhibitory ligand, and more particularly, to the detailed crystallographic data obtained from said co-crystallization which is disclosed herein. The invention also relates to methods of using the crystal structure and x-ray crystallographic coordinates of the apo-HDLP and

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inhibitor-bound HDLP to design, isolate and screen compounds which bind to and inhibit the active site of HDLP and HDLP-related proteins, such as those proteins belonging to the HDAC family, including HDAC1.

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Background of the Invention

The reversible modification of histones by acetylation is associated with changes in nucleosome conformation and chromatin structure, and plays an important role in the regulation of gene expression (reviewed in Davie and Chadee, 1998, J. Cell Biochem. Suppl. 30-31:203-213). The histone acetylase and deacetylase enzymes that carry out these modifications are involved in many cellular processes such as cell cycle progression and differentiation, and their deregulation is associated with several types of human cancer (reviewed in Kouzarides, 1999, Curr. Opin. Genet. Dev. 9:40-48; Hassig et al., 1997, Chem. Biol. 4:783-789; Fenrick and Heibert, 1998, J. Cell. Biochem. Suppl. 30-31:194-202).

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Recently, several experimental antitumor compounds, such as trichostatin A (TSA), trapoxin, suberoylanilide hydroxamic acid (SAHA), and phenylbutyrate have been shown to act, at least in part, by inhibiting histone deacetylases. Richon et al., 1998, Proc. Natl. Acad. Sci., USA 95:3003-3007; Yoshida et al., 1990, J. Biol. Chem. 265:17174-17179; Kijima et al., 1993, J. Biol. Chem. 268:22429-22435. Additionally, diallyl sulfide and related molecules (Lea et al., 1999, Int. J. Oncol. 2:347-352), oxamflatin (Kim et al., 1999, Oncogene 15:2461-2470), MS-27-275, a synthetic benzamide derivative (Saito et al., 1999, Proc. Natl. Acad. Sci. 96:4592-4597),

butarate derivatives (Lea and Tulsyan, 1995, Anticancer Res. 15:879-883), FR901228 (Nokajima et al., 1998, Exp. Cell Res. 241:126-133), depudecin (Kwon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3356-3361) and m-carboxysinnamic acid bishydroxamide (CBHA; Richon et al., Proc. Natl. Acad. Sci. USA 95:3003-3007) have been shown to inhibit histone deacetylases. In vitro, these compounds can inhibit the growth of fibroblast cells by causing cell cycle arrest in the G1 and G2 phases (Richon et al., 1996, Proc. Natl. Acad. USA <u>93</u>:5705-5708; Kim et al., 1999, 18:2461-2470; Yoshida et al., 1995, Bioessays 17:423-430; Yoshida & Beppu, 1988, Exp. Cell. Res. 177:122-131), and can the terminal differentiation and lead to transforming potential of a variety of transformed cell Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; Kim et al., 1999, Oncogene 18:2461-2470; Yoshida et al., 1987, Cancer Res. 47:3688-3691. phenylbutyrate is effective in the treatment of acute promyelocytic leukemia in conjunction with retinoic acid. Warrell et al., 1998, J. Natl. Cancer Inst. 90:1621-1625. SAHA is effective in preventing the formation of mammary tumors in rats, and lung tumors in mice. Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., Cancer Res., submitted.

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Histone deacetylases catalyze the removal of acetyl groups from the e-amino groups of lysine residues clustered near the N-terminus of nucleosomal histones, and this process is associated with transcriptional repression (reviewed in Struhl, 1998, Genes Dev. 12:599-606). Deletion of the yeast histone deacetylase gene, rpd3, or its pharmacological

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inactivation with trichostatin A reduces the transcriptional repression in a subset of promoters, such as those of Ume6-regulated genes. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127. This is accompanied by the increased acetylation of H4 histones in the repressed promoter and its vicinity, but has no effect on histones at promoter distal regions. Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127; Rundlett et al., 1998, Nature 392:831-835.

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Histone deacetylases are recruited to specific promoters by associating with DNA-binding transcriptional repressors, either directly or through co-repressors that bridge the deacetylase to the transcriptional repressors. For example, the Mad and Ume6 repressors bind to the co-repressor Sin3A (Laherty et al., 1997, Cell 89:349-356; Hassig et al., 1997, Cell 89:341-347; Kadosh & Struhl, 1997, Cell 89:365-371), and the nuclear receptors bind N-CoR and the related SMRT co-repressors. Nagy et al., 1997, Cell 89:373-380; Alland et al, 1997, Nature 387:49-55; Heinzel et al, 1997, Nature 387:43-48.

The deregulation of histone deacetylase recruitment appears to be one of the mechanisms through which these enzymes contribute to tumorigenesis. In acute promyelocytic leukemia (APL), chromosomal translocations fuse the retinoic acid receptor- α (RAR α) to either PLZF or to PML. These fusion oncoproteins have aberrant transcriptional repression activity resulting, in part, through the recruitment of a co-repressor and, in turn, HDACs. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814. Treatment of PLZF-RAR α APL cells with TSA enhances their

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responsiveness to retinoic acid-induced differentiation. Grignani et al, 1998, Nature 391:815-818; Lin et al., 1998, Nature 391:811-814.

The histone deacetylases comprise a large family of 5 proteins, conserved from yeast to man, and are divided into two related classes. Class I is characterized by human HDAC1, 2, 3 (Taunton et al., 1996, Science 272:408-411; Yang et al., 1996, Proc. Natl. Acad. Sci. USA 93:12845-12850; Emiliani et al., 1998, Proc. Natl. Acad. Sci. USA 95:2795-10 2800), and yeast RPD3 (Videl & Gaber, 1991, Mol. Cell. Biol. 11:6317-6327), and class II by the human HDAC4, 5, 6 (Grozinger et al., 1999, Proc. Natl. Acad. Sci. USA 96:4868-4873; Fischle, et al., 1999, J. Biol. Chem. 274:11713-11720), and yeast HDA1 (Rundlett et al., 1996, Proc. Natl. 15 Acad. Sci. USA <u>93</u>:14503-14508). The two classes share a ~390 amino acid region of sequence similarity, comprising the deacetylase core, but are divergent outside this region. The histone deacetylase genes belong to an even larger superfamily (Leipe & Landsman, 1997, Nucleic Acids Res. 20 the prokaryotic that contains 25:3693-3697) utilization proteins (AcuC; 28.1% sequence identity to HDAC1), and the prokaryotic acetylpolyamine amidohydrolases (APAH; 15.0 % sequence identity to HDAC1). The enzymatic activity of AcuC is not clear, but its disruption reduces 25 the ability of B. subtilis to breakdown acetoin and utilize it as a carbon source. Grundy et al., 1993, Mol. Microbiol. 10:259-271. APAHs catalyze the deacetylation of polyamines by cleaving a non-peptide amide bond (reviewed in Leipe & Landsman, 1997, Nucleic Acids Res. 25:3693-3697). 30

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It is useful to address the questions of how HDACs and HDACrelated proteins catalyze the deacetylation of histones and how the above-referenced compounds, particularly those compounds with antitumor activity, inhibit this activity in order to better understand the mechanism of inhibition of HDACs and to facilitate discovery of additional useful compounds which may inhibit this activity. To this end, the present invention has determined the three dimensional structure of a HDAC1-like protein from the thermophilic bacterium Aquifex aeolicus, herein after HDLP. The determination of the nucleic acid coding sequence of HDLP was described by Deckert et al., 1998, Nature 392:353-358. The encoded 375 residue protein, whose sequence was determined from the nucleic acid encoding sequence, shares 35.2% amino acid sequence identity with HDAC1, deacetylates histones in vitro, and is inhibited by TSA, SAHA and several The determination of the threeother HDAC inhibitors. dimensional structure of HDLP is useful in the design, identification and screening of new HDAC family inhibitory compounds which are useful for the inhibition of cell growth both in vivo and in vitro.

Summary of the Invention

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In general, it is the object of the present invention to provide detailed three-dimensional structural information for a family of proteins known as histone deacetylases (HDAC), and particularly a homologue from the hyperthermophilic bacterium Aquifex aeolicus HDLP (histone deacetylase-like protein) which shares 35.2 % sequence identity with human histone deacetylase (HDAC1). It is also an object of the present invention to provide three-

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dimensional structural information of an HDLP bound to an inhibitory compound.

In one embodiment of the invention, three-dimensional structure information is obtained from a crystal of wildtype HDLP (SEQ ID NO:1) (the nucleic acid encoding wild-type HDLP is SEQ ID NO:2). In a further embodiment of the invention, three-dimensional information is obtained from a mutant HDLP comprising two mutations (1) cysteine 75 to a serine and (2) cysteine 77 to a serine (Cys75Ser/Cys77Ser double mutant; SEQ ID NO:3) (the nucleic acid encoding HDLP Cys75Ser/Cys77Ser double mutant is SEQ ID NO:4). invention facilitates mutant of the present determination of three-dimensional structural information of HDLP bound to a zinc atom at its zinc atom-binding site.

In a preferred embodiment of the invention, the threedimensional structural information is obtained from a cocrystal of a protein-inhibitor compound complex that comprises HDLP or HDLP Cys75Ser/Cys77Ser double mutant and trichostatin A (TSA). In another preferred embodiment of the invention the three-dimensional structural information is obtained from a co-crystal of a protein-inhibitor HDLP comprises HDLP orcomplex that compound and suberoylanilide Cys75Ser/Cys77Ser double mutant hydroxamic acid (SAHA). Any HDLP or HDLP-related protein (e.g. HDAC) inhibitor compound that may be co-crystallized with HDLP may be used to form a co-crystal of the present invention.

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The protein crystals and protein-inhibitory complex cocrystals of the present invention diffract to a high

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resolution limit of at least equal to or greater than 4 angstrom (Å). In a preferred embodiment, the protein crystals and protein-inhibitory complex co-crystals of the present invention diffract to a high resolution limit of greater than 2.5 Å.

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A crystal of the present invention may take a variety of forms, all of which are contemplated by the present invention. In a preferred embodiment, the crystal has a space group of C2 with one molecule in the asymmetric unit and with unit dimensions of a = 51.4 Å, b = 93.8 Å, 78.7 Å and $\beta = 96.9^{\circ}$ (see, e.g., Example 2, below). another preferred embodiment, the crystal has a space group of $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a = 53.4 Å, b = 94.4 Å, c = 156.3 Å (see, e.g., Example 2, below). The HDLP structure comprises a parallel β sheet with α helices packing against both faces. At one end of the β sheet, the HDLP has a narrow, tube-like pocket formed by several well-ordered loops. The walls of the pocket are lined with hydrophobic residues and there is a zinc binding site and several polar side chains at the The inhibitory compounds of the bottom of the pocket. present invention bind in the pocket.

The three-dimensional structural information obtained from crystals of HDLP, HDLP Cys75Ser/Cys77Ser double mutant, HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc atom, HDLP comprising an inhibitory compound such as TSA or SAHA, and HDLP Cys75Ser/Cys77Ser double mutant comprising an inhibitor compound such as TSA or SAHA may be employed to solve the structure of any HDLP-related protein (e.g. HDAC) crystal,

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or any mutant HDLP-related protein and particularly any wild type or mutant of HDLP-related protein complexed with a ligand, including a substrate or inhibitor compound. If the crystals are in a different space group than the known structure, molecular replacement may be employed to solve the structure, or if the crystals are in the same space group, refinement and difference fourier methods may be employed. The structure of HDLP-related proteins (e.g. HDAC1) comprise no greater than a 2.0 Å root mean square deviation (rmsd) in the positions of the C α atoms for at least 50% or more of the amino acids of the full-length HDLP structure.

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The present invention also provides a nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant having the amino acid sequence of SEQ ID NO:3 and the nucleic acid sequence of SEQ ID NO:4. It is also contemplated by the invention that mutations be made in HDLP-related proteins at cysteine residues, as with the Cys75Ser/Cys77Ser double mutant, in order to facilitate the determination of the structure of said proteins bound to a zinc atom. Additionally, the present invention provides expression vectors which comprise the nucleic acid molecule encoding an HDLP Cys75Ser/Cys77Ser double mutant encoded by the sequence represented by SEQ ID NO:4 operatively linked to expression control sequences.

It is another object of the present invention to provide methods for the design, identification and screening of potential inhibitor compounds of the HDLP/HDAC family. In a preferred embodiment the method for the rational design,

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identification and screening of potential inhibitor compounds for HDLP and HDLP-related proteins (e.g. HDACs) comprising deacetylase activity comprises the steps of: (a) using a three-dimensional structure of an HDLP as defined by the atomic coordinates of the present invention; employing said three-dimensional structure to design or select said potential inhibitor compound; (c) synthesizing and/or selecting said potential inhibitor; (d) contacting said potential inhibitor compound with said enzyme in the presence of acetylated substrate; and (e) determining the percent inhibition of deacetylase activity to determine the inhibitory activity of said potential inhibitor compound. In a further preferred embodiment, the binding properties of said rationally designed inhibitory compound determined by a method comprising the steps of: (a) forming a complex comprising said inhibitory compound and HDLP or a HDLP-related protein, (b) co-crystallizing said inhibitory determining said compound-HDLP complex; (c) dimensional structure of said co-crystal through molecular replacement or refinement and difference fourier with the molecular coordinates of HDLP as defined by the present invention; and (d) analyzing the three-dimensional structure to determine the binding characteristics of said potential inhibitor compound.

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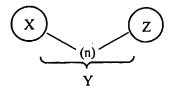
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It is a further object of the present invention to identify a defined class of HDLP/HDAC family inhibitor compounds. The HDLP/HDAC family inhibitor compounds of the present invention are represented by formula (I):

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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises and active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and may further bind to a zinc atom.

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Brief Description of the Drawings

Figure 1 is a table listing the statistics from the X-ray crystallographic analysis of a HDLP crystal, a HDLP-TSA cocrystal, and a HDLP-SAHA co-crystal.

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Figure 2 shows an alignment of various HDAC homologues with percent sequence identity depicted.

Figure 3 shows a graph indicating the histone deacetylase activity of HDLP and HDAC1 and the inhibition of HDLP and HDAC1 by the inhibitors TSA and HC-toxin.

Figure 4 shows (A & B) a schematic representation of the $HDLP-Zn^{2+}-TSA$ complex in two approximately orthogonal views, (C) a topology diagram of HDLP indicating the regions of homology with HDAC1, and (D) a close-up schematic representation of the $HDLP-Zn^{2+}-SAHA$ complex.

Figure 5 shows (A) a schematic representation of a slice through a surface representation of HDLP with the pocket internal cavities and position of the β sheet indicated, (B) a schematic representation of a close-up view of the active site looking down into the pocket in an orientation similar to Figure 4B.

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Figure 6 shows (A) a space-filling representation of TSA in the active site pocket, (B) a closeup stereo view of the structure of the $HDLP-ZN^{2+}-TSA$ complex in a similar orientation to Figure 4B, and (C) a schematic representation of the HDLP-TSA interactions.

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Figure 7 shows (A) a schematic representation of the regions of homology shared between HDLP and HDAC1 in an orientation similar to that of Figure 4A, and (B) a detailed schematic representation of the homology shared in the pocket and internal cavity between HDLP and HDAC1 in an orientation similar to that of Figure 4B.

Figure 8 shows a schematic representation of the proposed catalytic mechanism for the deacetylation of acetylated lysine.

Figure 9 shows a schematic representation of a space filling diagram showing the conserved amino acids in the active site and nearby grooves.

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Figure 10 is the nucleic acid sequence of HDLP from Aquifex aeolicus (SEQ ID NO. 2).

Figure 11 is the amino acid sequence of full length HDLP from Aquifex aeolicus (SEQ ID NO. 1).

Figure 12 is the nucleic acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 6).

25 Figure 13 is the amino acid sequence of the HDLP active site mutant Tyr297Phe (SEQ ID NO. 5).

Figure 14 is the nucleic acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 4).

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Figure 15 is the amino acid sequence of a double mutant of HDLP from Aquifex aeolicus comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO. 3).

Figure 16-1 to 16-49 lists the atomic structure coordinates for HDLP as derived by X-ray diffraction from a crystal of HDLP.

Figure 17-1 to 17-49 lists the atomic structure coordinates

for HDLP Cys75Ser/Cys77Ser double mutant comprising a zinc

atom in the active site as derived by X-ray diffraction from

a crystal of the HDLP Cys75Ser/Cys77Ser double mutant.

Figure 18-1 to 18-99 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with TSA.

Figure 19-1 to 19-48 lists the atomic structure coordinates for HDLP Cys75Ser/Cys77Ser double mutant as derived by X-ray diffraction from a co-crystal of HDLP complexed with SAHA.

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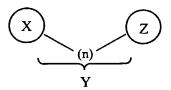
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Detailed Description of the Invention

The present invention provides crystals of a histone deacetylase (HDAC) homologue grown in the presence and absence of a compound capable of inhibiting the histone deacetylase activity of said HDAC homologue. As referred to herein, a HDAC homologue (as well as a HDLP-related protein) is any protein molecule having (a) greater than 15% sequence identity to over the 375 amino acid residues of HDLP; (b) having no more than twenty insertions or deletions for a total of no more than 100 amino acids; and (c) deacetylase activity. Sequence identity is calculated by the program DNAstar[™] using the identity matrix weighing scheme clustal method (DNAstar program, Madison, WI).

A HDLP/HDAC inhibitor compound, as used herein, refers to any compound represented by Formula (I):

(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of tyrosine, proline and leucine; Y comprises an aliphatic chain group from about 5 to about 10 Å, preferably 7Å, which binds to at least one amino acid selected from the group consisting of phenylalanine and glycine; and Z comprises a active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and which may further bind to a zinc atom. The HDAC inhibitory compounds of the present

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invention can inhibit greater than 50% of the histone deacetylase activity of a HDAC homologue or a HDLP-related protein.

To grow the crystals of the present invention, the HDAC and HDAC-inhibitory compound complex are purified to greater than 80% total protein and more preferably purified to greater than 90% total protein. For expression and purification purposes, the full-length HDLP (Genbank accession number AE000719) may be subcloned from Aquifex aeolicus chromosomal DNA preparation by the polymerase chain reaction (PCR) and inserted into an expression vector.

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A large number of vector-host systems known in the art may be used. Possible vectors include, but are not limited to, plasmids or modified viruses, but the vector system must be compatible with the host cell used. Examples of vectors include E. coli bacteriophages such as lambda derivatives, or plasmids such as pBR322 derivatives or pUC plasmid e.g., pGEX vectors derivatives, (Amersham-Pharmacia, Piscataway, New Jersey), pET vectors (Novagen, Madison, WI), pmal-c vectors (Amersham-Pharmacia, Piscataway, New Jersey), pFLAG vectors (Chiang and Roeder, 1993, Pept. Res. 6:62-64), baculovirus vectors (Invitrogen, Carlsbad, CA; Pharmingen, The insertion into a cloning vector San Diego, CA), etc. can, for example, be accomplished by ligating the DNA fragment into a cloning vector which has complementary cohesive termini, by blunt end ligation if no complementary cohesive termini are available or by through nucleotide linkers using techniques standard in the art. Ausubel et al. (eds.), Current Protocols in Molecular

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Biology, (1992). Recombinant vectors comprising the nucleic acid of interest may then be introduced into a host cell compatible with the vector (e.g. E. coli, insect cells, mammalian cells, etc.) via transformation, transfection, infection, electroporation, etc. The nucleic acid may also be placed in a shuttle vector which may be cloned and propagated to large quantities in bacteria and then introduced into a eukaryotic cell host for expression. The vector systems of the present invention may provide expression control sequences and may allow for the expression of proteins in vitro.

In a preferred embodiment, the full length HDLP (SEQ ID NO:2) is subcloned from Aquifex aeolicus chromosomal DNA preparation into pGEX4T3 (Amersham-Pharmacia, Piscataway, New Jersey). In order to construct a double mutant comprising a Cys75Ser and Cys77Ser mutation (SEQ ID NO:4), and to construct the HDLP active site mutant Tyr297Phe (SEQ ID NO:5 and SEQ ID NO:6), PCR site directed mutagenesis may be employed with verification by DNA sequencing by methods known to those skilled in the art (see, e.g., Example 1 below). The mutants of the present invention may be subcloned into a suitable expression vector and introduced into a host cell for protein production, as described above.

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The HDLP nucleic acids of the present invention may be subcloned into an expression vector to create an expression construct such that the resultant HDLP molecule which is produced comprises a fusion protein wherein said fusion protein comprises a tag for ease of purification. As referred to herein, a "tag" is any additional amino acids

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which are provided in a protein either c-terminally, nterminally or internally for the ease of purification, for the improvement of production or for any other purpose which may facilitate the goals of the present invention (e.g. to achieve higher levels of production and/or purification). Such tags include tags known to those skilled in the art to be useful in purification such as, but not limited to, his tag, glutathione-s-transferase tag, flag tag, mbp (maltose binding protein) tag, etc. In a preferred embodiment, the wild-type and mutant HDLPs of the present invention are tagged with glutathione-s-transferase (see Example 1 below). In another preferred embodiment, HDAC1 is flag tagged (see Example 1 below). Such tagged proteins may also be engineered to comprise a cleavage site, such as a thrombin, enterokinase or factor X cleavage site, for ease of removal of the tag before, during or after purification. systems which provide a tag and a cleavage site for removal of the tag are particularly useful to make the expression constructs of the present invention.

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The tagged HDLPs and HDACs of the present invention may be purified by immuno-affinity or conventional chromatography, including but not limited to, chromatography employing the glutathione-sepharose™ (Amersham-Pharmacia, following: Piscataway, New Jersey) or an equivalent resin, nickel or cobalt-purification resins, anion exchange chromatography, cation exchange chromatography, hydrophobic resins, gel antiflag epitope resin, reverse filtration, chromatography, etc. After purification, the HDLP and HDLPinhibitor compound complex may be concentrated to greater than 1 mg/ml for crystallization purposes. In a preferred HDLP-inhibitor complexes HDLP and are embodiment

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concentrated to greater than 10 mg/ml for crystallization and in a particularly preferred embodiment, HDLP and HDLP-inhibitor complexes are concentrated to greater than 20 mg/ml.

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In order to determine whether the purified HDLPs of the present invention demonstrate histone deacetylase activity, the purified HDLPs and also any HDLP-related protein may be assayed by any method known to those skilled in the art for the determination of said activity. In a preferred embodiment, the purified HDLPs of the present invention are incubated in the presence of [3H] acetyl-labeled histone substrate (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844) in a buffer suitable for detection of histone deacetylase activity (see Example 3 below); stopping the reaction; extracting the released acetate and measuring said released acetate, as described by Henzel et al. (J. Biol. Chem. 266:21936-21942 (1991); Example 3 below). preferred embodiment, the HDLPs of the present invention are inclubated in the presence of ZnCl2 in order to obtain histone deacetylase activity therefrom (Example 3 below).

In another embodiment, the crystals of the present invention comprise purified wild-type HDLP (SEQ ID NO:1) and are grown at room temperature by the hanging-drop vapor-diffusion method from a crystallization solution comprising one or more precipitants selected from the group consisting of isopropanol, polyethylene glycol, and tert butanol (see Example 2 below). The crystallization solution may further comprise one or more salts including salts selected from the group consisting of NaCl and KCl, and one or more buffers

including buffers selected from the group consisting of Tris (tris(hydroxymethyl)aminomethane and bis-tris propane-Cl (1,3-bis[tris(hydroxymethyl)methyl-amino] propane) (see Example 2 below). The pH of the crystallization solution is preferably between pH 5 to 9, although other pH values are also contemplated by the present invention (see Example 2 below).

Any crystallization technique known to those skilled in the art may be employed to obtain the crystals of the present invention, including, but not limited to, batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and micro dialysis. Seeding of the crystals in some instances may be required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used.

The crystals of the present invention may form in the space group C2 with one molecule in the asymmetric unit and with unit dimensions of a=51.4 Å, b=93.8 Å, c=78.7 Å and $\beta=96.9^{\circ}$ (see Example 2 below). The crystals of the present invention may also form in the space group $P2_12_12_1$ with two molecules in the asymmetric unit and with unit dimensions of a=53.4 Å, b=94.4 Å, c=156.3 Å (see Example 2 below). However, the present invention contemplates crystals which form in any space group including, but not limited to, C2, $P2_1$, $P2_12_12_1$, $P3_121$, $P4_32_12_1$, and $C222_1$. The crystals diffract to a resolution greater than 4 Å, preferably greater than 2.5 Å.

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To collect diffraction data from the crystals of the present

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invention, the crystals may be flash-frozen in the crystallization buffer employed for the growth of said crystals, however with preferably higher precipitant concentration (see, e.g., Example 2 below). For example, but not by way of limitation, if the precipitant used was 28% PEG 1500, the crystals may be flash frozen in the same crystallization solution employed for said crystal growth wherein the concentration of the precipitant is increased to 35% (see Example 2 below). If the precipitant is not a sufficient cryoprotectant (i.e. a glass is not formed upon cryoprotectants (e.g. glycerol, low flash-freezing), molecular weight PEGs, alcohols, etc) may be added to the solution in order to achieve glass formation upon flashfreezing, providing the cryoprotectant is compatible with preserving the integrity of the crystals. The flash-frozen crystals are maintained at a temperature of less than -110°C and preferably less than -150°C during the collection of the crystallographic data by X-ray diffraction. diffraction data may be processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method Ensemble. 276:307-326) but any method known to those skilled in the art may be used to process the X-ray diffraction data.

In order to determine the atomic structure of HDLP according to the present invention, multiple isomorphous replacement (MIR) analysis, model building and refinement may be performed. For MIR analysis, the crystals may be soaked in heavy-atoms to produce heavy atom derivatives necessary for MIR analysis. As used herein, heavy atom derivative or derivitization refers to the method of producing a chemically modified form of a protein or protein complex

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crystal wherein said protein is specifically bound to a heavy atom within the crystal. In practice a crystal is soaked in a solution containing heavy metal atoms or salts, or organometallic compounds, e.g., lead chloride, gold cyanide, thimerosal, lead acetate, uranyl acetate, mercury chloride, gold chloride, etc, which can diffuse through the crystal and bind specifically to the protein. The location(s) of the bound heavy metal atom(s) or salts can be determined by X-ray diffraction analysis of the soaked This information is used to generate MIR phase crystal. information which is used to construct the three-dimensional structure of the crystallized HDLPs and HDLP-related proteins of the present invention. In a preferred embodiment, the heavy atoms comprise thimerosal, KAu(CN)2 and Pb(Me)₃OAc (see Example 2 below). The MIR phases may be calculated by any program known to those skilled in the art and preferably with the program MLPHARE (The CCP4 suite: Programs for computational crystallography, 1994, Crystallogr. D. 50:760-763) and may also use the anomalous diffraction signal from the thimerosal derivative. preferred embodiment, the MIR phases were calculated at 2.5 Å and have a mean figure of merit of 0.55 (see Figure 19 and The phases may be improved where Example 2 below). necessary by solvent flattening by methods known to those skilled in the art including, but not limited to, through the use of the program DM (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D <u>50</u>:760-763).

Thereafter, an initial model of the three-dimensional structure may be built using the program O (Jones et al.,

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1991, Acta Crystallogr. A $\underline{47}$:110-119). The interpretation and building of the structure may be further facilitated by use of the program CNS (Brunger et al., 1998, Acta Crystallogr. D $\underline{54}$:905-921).

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For the determination of the HDLP-inhibitor compound complex structure, if the space group of the HDLP-inhibitor compound complex crystal is different, molecular replacement may be employed using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure whose structure may be determined as described above and below in Example 2. the space group of the HDLP-inhibitor compound crystals is the same, then rigid body refinement and difference fourier may be employed to solve the structure using a known structure of apo-HDLP (as referred to herein, apo-HDLP or apo-HDAC is the enzyme which is not complexed with an inhibitor compound) or any known HDLP/inhibitor complex structure.

The term "molecular replacement" refers to a method that involves generating a preliminary model of the three-dimensional structure of the HDLP crystals of the present invention whose structure coordinates are unknown prior to the employment of molecular replacement. Molecular replacement is achieved by orienting and positioning a molecule whose structure coordinates are known (in this case the previously determined apo-HDLP) within the unit cell as defined by the X-ray diffraction pattern obtained from an

HDLP or HDLP-related protein crystal whose structure is

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unknown so as to best account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This in turn can be subject to any of several forms of refinement to provide a final, accurate structure.

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Any method known to the skilled artisan may be employed to determine the structure by molecular replacement. example, the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D. 50:760-763) may be employed to determine the structure of an unknown histone deacetylase +/- an inhibitor by molecular replacement using the apo-HDLP coordinates (Figure 16). For the structure determination of the inhibitory compound TSA, the structure of TSA was obtained from the Cambridge (Refcode TRCHST, Structural Database http://www.ccdc.cam.ac.uk >>) may be employed to define the stereochemical restraints used in the refinement with the program CNS (Brunger et al., 1998, Acta Crystallogr. D <u>54</u>:905-921).

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP are useful for solving the structure of crystallized proteins which belong to the HDAC family by molecular replacement. Similarly, any structure of a crystallized protein which is thought to be similar in structure based on function or sequence similarity or identity to HDLP may be solved by molecular replacement with the HDLP structural

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information of the present invention. The structure of HDLP-related proteins as determined by molecular replacement as described above and in Example 2 below, comprise a root mean square deviation (rmsd) of no greater than 2.0 Å in the positions of $C\alpha$ atoms for at least 50% or more of the amino acids of the structure over the 375 residues of full-length HDLP. Such a rmsd may be expected based on the amino acid sequence identity. Chothia & Lesk, 1986, Embo J. $\underline{5}$:823-826.

The refined three-dimensional HDLP structures of the present invention, specifically apo-HDLP, Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site, HDLP/TSA complex comprising a zinc atom in the active site, and HDLP/SAHA complex comprising a zinc atom in the active site, are represented by the atomic coordinates set forth in Figures 16 to 19 respectively. The refined model for apo-HDLP comprising amino acids 1-375 consists of wild-type HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution Å. Similarly, the refined model 1.8 Cys75Ser/Cys77Ser double mutant HDLP comprising a zinc atom in the active site also consists of residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered and was determined to a resolution of 2.0 Å. The refined model for the HDLP/TSA complex comprising a zinc atom in the active site consists of the Cys75Ser/Cys77Ser double mutant HDLP residues 2 to 373 with residues 1, 374 and 375 not modeled and presumed disordered, has TSA in the binding pocket and was determined to a resolution of 2.1 Å. HDLP/SAHA complex is similar to the HDLP/TSA complex but has SAHA in the binding pocket and was determined to a resolution of 2.5 Å.

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For the purposes of further describing the structure of HDLP and HDLP-related proteins, including, but not limited to, HDACs, from the data obtained from the HDLP crystals of the present invention, the definition of the following terms is provided:

The term " β sheet" refers to two or more polypeptide chains (or β strands) that run alongside each other and are linked in a regular manner by hydrogen bonds between the main chain C=O and N-H groups. Therefore all hydrogen bonds in a beta-sheet are between different segments of polypeptide. Most β -sheets in proteins are all-parallel (protein interiors) or all-antiparallel (one side facing solvent, the other facing the hydrophobic core). Hydrogen bonds in antiparallel sheets are perpendicular to the chain direction and spaced evenly as pairs between strands. Hydrogen bonds in parallel sheets are slanted with respect to the chain direction and spaced evenly between strands.

The term " α helix" refers to the most abundant helical conformation found in globular proteins. The average length of an α helix is 10 residues. In an α helix, all amide protons point toward the N-terminus and all carbonyl oxygens point toward the C-terminus. The repeating nature of the phi, psi pairs ensure this orientation. Hydrogen bonds within an α helix also display a repeating pattern in which the backbone C=O of residue X (wherein X refers to any amino acid) hydrogen bonds to the backbone HN of residue X+4. The α helix is a coiled structure characterized by 3.6 residues per turn, and translating along its axis 1.5 Å per amino acid. Thus the pitch is 3.6x1.5 or 5.4 Å. The screw sense of alpha helices is always right-handed.

The term "loop" refers to any other conformation of amino acids (i.e. not a helix, strand or sheet). Additionally, a loop may contain bond interactions between amino acid side chains, but not in a repetitive, regular fashion.

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Amino acid residues in peptides shall herein after be abbreviated as follows: Phenylalanine is Phe or F; Leucine is Leu or L; Isoleucine is Ile or I; Methionine is Met or M; Valine is Val or V; Serine is Ser or S; Proline is Pro or P; Threonine is Thr or T; Alanine is Ala or A; Tyrosine is Tyr or Y; Histidine is His or H; Glutamine is Gln or Q; Asparagine is Asn or N; Lysine is Lys or K; Aspartic Acid is Asp or D; Glutamic Acid is Glu or E; Cysteine is Cys or C; Tryptophan is Trp or W; Arginine is Arg or R; and Glycine is Gly or G. For further description of amino acids, please refer to Proteins: Structure and Molecular Properties by Creighton, T.E., W.H. Freeman & Co., New York 1983.

The term "positively charged amino acid" refers to any amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged amino acids are Arg, Lys and His. The term "negatively charged amino acid" refers to any amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged amino acids are Asp and Glu. The term "hydrophobic amino acid" refers to any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of hydrophobic amino acids are Ala, Leu, Ile, Gly, Val, Pro, Phe, Trp and Met. The term "hydrophilic amino acid" refers to any amino acid having an uncharged, polar side chain that is

relatively soluble in water. Examples of hydrophilic amino acids are Ser, Thr, Tyr, Asp, Gln, and Cys. The term "aromatic amino acid" refers to any amino acid comprising a ring structure. Examples of aromatic amino acids are His, Phe, Trp and Tyr.

The term "charge relay system" refers to a His-Asp arrangement as described by Fersht & Sperling, 1973, J. Mol. Biol. 74:137-149; Blow et al., 1969, Nature 221:337-340.

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information obtained from the three-dimensional The structures of the present invention reveal that HDLP has a single-domain structure that belongs to the open α/β class of folds (see, e.g., Branden, 1980, Q. Rev. Biophys. 13:317-38). Two orthogonal views of the overall three-15 dimensional structure of HDLP are depicted in Figure 4A and The HDLP structure has a central eight-stranded parallel β sheet (strands arranged as $\beta 2 - \beta 1 - \beta 3 - \beta 8 - \beta 7 - \beta 4 - \beta 5$ and sixteen α helices (labeled α 1 through α 16 respectively). See Figure 4C. Four of the helices pack on 20 either face of the β sheet (α 7, α 8, α 9, α 10 and α 11, α 12, α 13, α 14) forming the core α/β structure characteristic of this class of folds. Most of the remaining eight helices are positioned near one side of the β sheet, near stands β 2β1-β3-β8. Large, well defined loops (Loops L1-L7; Figure 25 4C) originate from the C-terminal ends of the β -strands. The extra helices and the large L1-L7 loops are associated with a significant extension of the structure beyond the core α/β motif. This extension of the structure gives rise to two prominent architectural features: a deep, narrow 30 pocket and an internal cavity adjacent to the pocket. These

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two architectural features comprise the active site (see Figure 5A). The structure of HDLP-related proteins (e.g. HDACs) may also comprise the conserved α/β structure characteristic.

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The term "active site" comprises any or all of the following sites in HDLP, the substrate binding site, the site where the cleavage of an acetyl group from a substrate occurs or the site where an inhibitor of the HDAC family or, more particularly, HDLP binds. The active site, as referred to herein, comprises Aspl66, Asp258, His170, Tyr297, His131, His132, Aspl68, Asp173, Phe141, Phe198, Leu265, Pro22 and Gly140, and also a metal bound at the bottom of the pocket by Asp173, Aspl68 and His defined by the coordinates listed in Figures 16 to 19 with an rmsd of 2.0 Å. The metal which binds at the bottom of the pocket will be a divalent cation selected from the group consisting of zinc, cobalt or manganese.

The deep narrow pocket has a tube-like shape with a depth of ~ 11 Å. The pocket opening constricts half way down to ~ 4.5 by 5.5 Å, and becomes wider at the bottom (see Figure 5A). The pocket and its immediate surroundings are made up of loops L1 through L7.

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The walls of the pocket are covered with side chains of hydrophobic and aromatic residues (Pro22, Tyr91 near the entrance; and Gly140, Phe141, Phe 198, Leu265 and Tyr297 further down; Figure 5B). For numbering of amino acids please refer to SEQ ID NO:1. Of particular interest are Phe141 and Phe198, whose phenyl groups face each other in

parallel at a distance of 7.5 Å, marking the most slender portion of the pocket (see Figure 5B). Of particular interest is that only one pocket residue differs in HDAC1 when the sequences are aligned (alignment may be accomplished using DNAstar™ MegAlign™ program, Madison, WI), this residue is Glu98 of HDAC1 which is Tyr91 in HDLP. The structure reveals that this residue in HDLP is mostly solvent exposed.

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Near the bottom of the pocket of the active site at its narrowest point, is located a zinc ion (see Figure 6A). In order to obtain the zinc in the structure, the crystals may be soaked in zinc (e.g. ZnCl₂) or co-crystalized in the presence of zinc. The zinc ion is coordinated by Asp168 (Oδ1, 2.1 Å), His170 (Nδ1, 2.1 Å), Asp258 (Oδ1, 1.9 Å) and a water molecule (2.5 Å). See Figure 5B and 6B. The amino acid residues that coordinate zinc are arranged in a tetrahedral geometry, but the position of the water molecule, which is also hydrogen bonded to His131, deviates from this geometry by ~25°.

In addition to the zinc ligands, the bottom of the pocket contains two histidine (His131 and His132), two aspartic acids (Asp166 and Asp173) and a tyrosine (Tyr297). See Figure 5B and 10B. Each of the histidines makes a hydrogen bond through its Nol to an aspartic acid carboxylate oxygen, with the oxygen located in the plane of the imidizole ring (Figure 5B). This His-Asp arrangement is characteristic of the charge relay system present in the active sites of serine proteases, where it serves to polarize the imidizole Ne and increase its basicity. Fersht & Sperling, 1973, J.

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Mol. Biol. <u>74</u>:137-149; Blow et al., 1969, Nature <u>221</u>:337-340.

The Asp166-His131 charge pair relay (hereafter referred to as "buried charged relay") is positioned even deeper in the pocket and more buried compared to the Asp173-His132 charge relay (hereafter referred to as "exposed charge relay") which is partially solvent exposed. The buried charge relay makes a hydrogen bond (2.6 Å) to the zinc-bound water molecule referred to above, and this hydrogen bond could contribute to the deviation of the water-zinc coordination from ideal geometry (Figure 5B). The exposed charge relay is directed to a point ~ 2.5 Å away from the water molecule and closer to the surface.

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Tyr 297 is positioned next to the zinc, opposite from where the two charge relay systems are located. The Tyr hydroxyl group lies 4.4 Å away from the zinc atom and has no interactions with the rest of the protein (Figure 5B). Next to Tyr297, there is an opening in the pocket wall, which leads to the adjacent internal cavity.

The floor of the internal cavity is made up of portions of the L3 and L7 loops as they emerge from the β strands, and the roof is made up by the $\alpha 1\text{-L} 1\text{-}\alpha 2$ segment. The L1 loop appears more flexible than other loops in the structure. This may allow the transient exchange of the cavity contents with the bulk solvent.

The cavity is lined primarily with hydrophobic residues and is particularly rich in glycine residues (Ala127, Gly128, Gly129, Met130, and Phe141 of L3; Gly293, Gly294, Gly295 and

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Gly296 of L7; and Tyr17, Pro22 and Leu23 of L1). There are only two charged residues in the cavity (Arg27 and His 21) and these are contributed by the L1 loop.

The cavity may provide space for the diffusion of the acetate product away from the catalytic center, which may otherwise be crowded and shielded during deacetylation from the solvent when the substrate is bound. Such a role for the cavity is supported by the observation that the cavity contains three water and two isopropanol molecules (from the crystallization buffer) in the 1.8 Å apo-protein structure. The cavity may also bind another cofactor, in addition to zinc, for the facilitation of the enzymatic activity of the HDLP. A proposed catalytic mechanism for deacetylation is provided in Figure 8.

The structure of HDLP as defined by the present invention, in conjunction with the HDAC1 sequence homology, shows that the 375-amino acid HDLP protein corresponds to the histone deacetylase catalytic core which is conserved across the HDAC family (see Figure 2). The 35.2% HDLP-HDAC1 sequence identity predicts structural similarity with a rmsd in $C\alpha$ positions of ~ 1.5 Å. Chothia and Lesk describe the relation between the divergence of sequence and structure of proteins in Embo J. 5:823-826 (1986). The 40residue C-terminus of HDLP is likely to have a divergent structure since this region has lower homology to HDAC1, although the α 16 helix in this region is part of the conserved open α/β core fold and HDAC1 is likely to comprise a similar helix. However divergent this C-terminal region may be, this region is outside the active site and is likely to not effect the structure of the active site. Beyond the

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C-terminus of the histone deacetylase catalytic core, HDAC family members are divergent in length and sequence. In the HDAC family, this region (amino acid residues ~390-482) is highly polar, populated with acidic residues, and is likely to be flexible or loosely folded.

The HDLP-HDAC homology maps primarily to the hydrophobic core and to the L1-L7 loops, with portions of the loops that make up the pocket and adjacent cavity having the highest level of amino acid residue sequence conservation (Figure 9A and 9B). Specifically, all of the polar residues in the active site (the zinc ligands, the two charge relay systems, and Tyr297) and the hydrophobic residues that make up the walls of the pocket (Gly140, Phe141, Phe198 and Leu265) are identical. Among the residues that make up the internal cavity, the ones closest to the active site are either identical or conservatively substituted (for example, Leu23 \rightarrow Met and Met130 \rightarrow Leu). Surface residues around the pocket are conserved to a lesser extent, but are still above 35% average sequence identity.

The information obtained from the inhibitor-bound HDLP complex crystal structures of the present invention reveal detailed information which is useful in the design, isolation, screening and determination of potential inhibitor compounds which may inhibit HDLP/HDAC family members. As described above, the HDLP structure consists of a parallel β sheet with α helices packing against both faces (Figure 4A, 4B, and 4C). At one end of the β sheet, 7 loops (L1-L7) form a narrow, tube-like pocket which are lined with hydrophobic residues and which comprise a zinc binding site, several polar side chains, including two Asp-His charge

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relay systems. Mutation of the zinc ligands and other polar residues at the pocket bottom reduces or eliminates the catalytic activity.

The present inventors found that mutation at the Tyr297Phe site reduced activity. See also, Hassig et al., 1998, Proc. Natl. Acad. Sci. USA 95:3519-3524; Kadosh & Struhl, 1998, Genes Dev. 12:797-805. The elimination of activity by mutation of these residues indicates that this region is the enzyme active site. Adjacent to the active site, there is an internal cavity that may provide space for the diffusion of the acetate reaction product. Homology at the active site between HDLP and HDAC1, as described above, indicates that they share structural and functional homology.

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The inhibitor compound, trichostatin A (TSA) (Tsuji et al., 1976, J. Antibiotics 29:1-6) binds HDLP by inserting its long aliphatic chain, which has a hydroxamic acid group at one end, into the pocket (Figure 6A, 6B and 6C). aliphatic chain makes multiple contacts in the well-like, hydrophobic portion of the pocket. The hydroxamic acid reaches the polar bottom of the pocket, where it coordinates the zinc in a bidentate fashion and also forms hydrogen bonds with the polar residues in the active site, including the two charge relay system histidines. The aromatic dimethylamino-phenyl group at the other end of the TSA chain makes contacts at the pocket entrance and serves to cap it. The amino acid residues of HDLP which contact TSA are conserved in HDAC, indicating that TSA binds and inhibits HDAC in a similar fashion to HDLP.

In the complex, the hydroxamic acid, most of the aliphatic chain and part of the dimethylamino-phenyl group of TSA are buried (60% of TSA's surface area; Figure 6A). The hydroxamic acid group binds the zinc in a bidentite fashion forming bonds through its carbonyl (2.4 Å) and hydroxyl groups (2.2 Å) resulting in a penta-coordinated Zn²+ (Figure 6B and 6C). The hydroxamic acid hydroxyl group replaces the water molecule that binds to the zinc in the apo-HDLP structure described above. The hydroxamic acid also hydrogen bonds with both charge relay system histidines (hydroxyl oxygen to His131 Ne2, 2.8 Å; and nitrogen to His132 Ne2, 2.8 Å), and the Tyr297 hydroxyl group (2.4 Å; Figure 6B and 6C).

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The 5-carbon long branched alkene chain of TSA fits snugly in the narrow portion of the pocket making multiple van der Waals contacts with all of the hydrophobic groups lining the pocket (Figure 6B and 6C). Near its center, the chain contains a methyl substituted carbon-carbon double bond which is sandwiched between the phenyl groups of the Phel41 and Phe98 at the tightest point of the pocket (Figure 6A and 6B). The length of the alkene chain appears optimal for spanning the length of the pocket, and allowing contacts both at the bottom and at the entrance of the pocket, although, the cap group of Formula (I) may provide length to span the pocket allowing for a shorter alkene chain (aliphatic chain).

At the entrance of the pocket, one face of the planar structure formed by the dimethylamino-phenyl and adjacent carbonyl groups of TSA makes contacts at the rim of the pocket (Pro22, Tyr91, Phel41; Figure 6B and 6C). This

packing is facilitated by the roughly 110° angle in the overall structure of TSA at the junction of the aliphatic chain and the dimethylamino-phenyl group (occurring at the sp³ hybridized C8 carbon). Upon TSA binding, the side chain of Tyr91, which is mostly solvent exposed, changes conformation to make space for the dimethylamino-phenyl group. This is the only change near the active site observed upon TSA binding.

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10 The hydroxamic acid group is a common motif in zinc metalloprotease inhibitors. See U.S. Patent No. 5,919,940 and 5,917,090; See also, Grams et al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 15 20:6912-6920. Like TSA, these inhibitors also coordinate the active site zinc in a bidentate fashion using their hydroxamate hyroxyl and carbonyl oxygens, replace the nucleophilic water molecule with their hydroxamate hydroxyl groups and form hydrogen bonds to the general base (Grams et 20 al., 1995, Biochemistry 34:14012-14020; Lovejoy et al., 1999, Nat. Struct. Biol. 6:217-221; and Holmes & Matthews, 1981, Biochemistry 20:6912-6920).

SAHA, which has a ~30-fold weaker inhibitory activity than

TSA (Richon et al., 1998, Proc. Natl. Acad. Sci. USA

95:3003-3007), binds HDLP similarly to TSA (see, e.g.,

Figure 4D). The SAHA hydroxamic acid group makes the same

contacts to the zinc and active site residues, and the

importance of these interactions is underscored by the loss

of activity of SAHA derivatives lacking the hydroxamic group

(Richon et al., 1998, Proc. Natl. Acad. Sci. USA 95:3003-

3007). The six-carbon long aliphatic chain of SAHA packs in the tube-like hydrophobic portion of the pocket. Compared to TSA however, SAHA's aliphatic chain packs less snugly and makes fewer van der waals contacts, in part, because SAHA lacks TSA's C15 methyl group branch. SAHA also lacks TSA's double bonds in this region, and this may lead to increased flexibility of the aliphatic chain. The cap group of SAHA consists of a phenyl-amino ketone group. In the crystal structure, the phenyl group has weak electron density, suggesting that it does not pack as well as the cap group of TSA. This may be due to the larger separation between the hydroxamic and cap groups of SAHA compared to TSA (compare TSA, Formula (II) and SAHA, Formula (III), below).

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25 (III)

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The determination of the structure of HDLP and HDLP bound to an inhibitory compound has enabled, for the first time, the identification of the active site of HDLP and of related HDLP proteins, such as proteins belonging to the HDAC family.

The three-dimensional structural information and the atomic coordinates associated with said structural information of HDLP bound to an inhibitory compound is useful in rational drug design providing for a method of identifying inhibitory compounds which bind to and inhibit the enzymatic activity of HDLP, HDAC family proteins and other histone deacetylaselike proteins related to HDLP. Said method for identifying said potential inhibitor for an enzyme comprising deacetylase activity comprises the steps of (a) using a three-dimensional structure of HDLP as defined by its atomic coordinates listed in Figure 16 to 19; (b) employing said three-dimensional structure to design or select said (c) synthesizing said potential potential inhibitor; inhibitor; (d) contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and (e) determining the ability of said inhibitor to inhibit said deacetylase activity.

The potential HDLP and HDLP-related (e.g. HDAC) inhibitors identified by the method of the present invention are represented by formula (I)

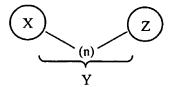
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(I)



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wherein X comprises a cap group which binds to at least one amino acid selected from the group consisting of proline and leucine; Y comprises an aliphatic chain group which binds to at least one amino acid selected from the group consisting of leucine, phenylalanine and glycine; and Z comprises an active site binding group which binds to at least one amino acid selected from the group consisting of aspartic acid, tyrosine and histidine and wherein Z may further bind to a zinc atom and with the provision that the compound of Formula (I) is not TSA, trapoxin, SAHA, SAHA derivatives described in U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5840,960 and 5,668,179.

The present invention permits the use of molecular design techniques to design, identify and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site of HDLP and HDLP-related proteins. The atomic coordinates of apo-HDLP and inhibitor-bound HDLP may be used in conjunction with computer modeling using a docking program such as GRAM, DOCK, HOOK or AUTODOCK (Dunbrack et al., 1997, Folding & Design 2:27-42) to identify potential inhibitors of HDLP and HDLP-related proteins (e.g. HDAC1). This procedure can include computer fitting of potential inhibitors to the active site of HDLP to ascertain how well the shape and the

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structure of the potential inhibitor complement the active site or to compare the potential inhibitors with the binding of TSA or SAHA in the active See Bugg et al, 1998, Scientific American December: 92-98; West et al., 1995, TIPS 16:67-74. potential inhibitors designed by modeling with a docking program conform to the general formula (I) as described Computer programs may also be employed to estimate above. the attraction, repulsion and stearic hindrance of the HDLP and potential inhibitor compound. Generally, the tighter the fit, the lower the stearic hindrances, the greater the attractive forces, and the greater the specificity which are important features for a specific inhibitory compound which is more likely to interact with HDLP and HDLP-related proteins rather than other classes of proteins. features are desired particularly where the inhibitory compound is a potential antitumor drug.

20 by visually inspecting the three-dimensional structure to determine more effective deacetylase inhibitors. This type of modeling may be referred to as "manual" drug design.

Manual drug design may employ visual inspection and analysis using a graphics visualization program such as "O" (Jones, T.A., Zhou, J.Y., Cowan, S.W., and Kjeldgaard, M., Improved method for building protein models in electron density maps and the location of errors in these models, Acta Crystallog., A47, 110-119.

Initially potential inhibitor compounds can be selected for their structural similarity to the X, Y and Z constituents

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of formula (I) by manual drug design. The structural analog thus designed can then be modified by computer modeling programs to better define the most likely effective candidates. Reduction of the number of potential candidates is useful as it may not be possible to synthesize and screen a countless number of variations compounds that may have some similarity to known inhibitory molecules. analysis has been shown effective in the development of HIV protease inhibitors (Lam et al., 1994, Science 263:380-384; Wlodawer et al., 1993, Ann. Rev. Biochem. 62:543-585; Appelt, 1993 Perspectives in Drug Discovery and Design 1:23-48; Erickson, 1993, Perspectives in Drug Discovery and Design 1:109-128. Alternatively, random screening of an small molecule library could lead to potential inhibitors whose inhibitory activity may then be analyzed by computer modeling as described above to better determine their effectiveness as inhibitors.

The compounds designed using the information of the present invention may be competitive or noncompetitive inhibitors. These designed inhibitors may bind to all or a portion of the active site of HDLP and may be more potent, more specific, less toxic and more effective than known inhibitors for HDLP and HDLP-related proteins, and particularly HDACs. The designed inhibitors may also be less potent but have a longer half life in vivo and/or in vitro and therefore be more effective at inhibiting histone deacetylase activity in vivo and/or in vivo for prolonged periods of time. Said designed inhibitors are useful to inhibit the histone deacetylase activity of HDLP and HDLP-related proteins (e.g. HDAC1), to inhibit cell growth in

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vitro and in vivo and may be particularly useful as antitumor agents.

The present invention also permits the use of molecular design techniques to computationally screen small molecule data bases for chemical entities or compounds that can bind to HDLP in a manner analogous to the TSA and SAHA as defined by the structure of the present invention. computational screening may identify various groups which may be defined as "X", "Y" or "Z" of formula (I) above and may be employed to synthesize the potential inhibitors of the present invention comprising formula (I). potential inhibitors may be assayed for histone deacetylase inhibitory activity in a histone deacetylase activity assay (see Example 3 below), may be co-crystallized with HDLP to the binding characteristics through X-ray determine crystallography techniques defined above (e.g. said cocrystal structure may be determined by molecular replacement to assess the binding characteristics of said potential inhibitor), or may be assessed based on binding activity by incubating said potential inhibitor with said HDLP, performing gel filtration to separate any free potential inhibitor to HDLP-bound inhibitor, and determining the amount of histone deacetylase activity of the inhibitorbound HDLP. To measure binding constants (e.g., Kd), methods known to those in the art may be employed such as Biacore™ analysis, isothermal titration calorimetry, Elisa with a known drug on the plate to show competitive binding, or by a deacetylase activity assay.

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The design of potential inhibitors of the present invention is further facilitated by reference to Figure 9, which is a surface representation figure that depicts the surface grooves. Analysis of such grooves gives insight into the constituents of the cap group of formula (I). The surface grooves are labeled groove A, groove A', groove B and groove C, into which additional cap groups may bind. The structure of HDLP bound to either TSA or SAHA shows that the cap groups of TSA and SAHA bind in groove A. By analysis of the amino acid sequence identity of HDLP and HDACs, Groove A is well conserved in HDACs, has a significant hydrophobic component, appears deep enough to allow for significant interactions and is also the largest of the four grooves. In addition to the dimethylamino phenyl group of the TSA, the A groove can fit approximately 200 daltons worth of groups (e.g. groove A could accommodate a naphthalene-like group after an appropriate spacer, etc.). Groove A, as referred to herein, is characterized by the following conserved residues of HDLP: His 21, Pro22, Lys24, Phe141, Leu265 and Phe335. The periphery of groove A comprises unconserved residues. Additionally, Groove A', as referred to herein, comprises primarily unconserved residues.

Groove B is immediately adjacent to the pocket. Of significance is that the bottom of groove B comprises the Nepsilon nitrogen of His170, which coordinates the zinc through its N-delta nitrogen. Significant binding energy may be achieved by contacting the Ne proton of His170 with a carboxylic acid or sulfate group. In addition, groove B may be large enough to fit a phenyl group, the face of which may comprise a partial negative charge which may pack over the N-epsilon proton of His170. The conserved residues of

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groove B, as referred to herein are: His170, Tyr196 and Leu265.

Groove C is not as well conserved as the other two grooves and the amino acid residues which comprise groove C are mostly polar and solvent exposed. Groove C, as referred to herein comprises the following conserved residues: Asn87, Gly140 and Phe198.

The compounds of the present invention are represented by formula (I):

(I)

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15 (x)

Examples for suitable X constituents wherein X comprises a cap group may be described in three categories, depending upon which surface of groove A, A', B and/or C they are targeted to. The cap group may comprise all three categories on the same compound. Of particular benefit may be replacing the cap group of TSA or SAHA with a large, rigid structure. Nonlimiting examples for suitable cap groups (X) of formula (I) which may bind in groove A are: (1) attaching a 1-3 methyl linker followed by a phenyl or naphthalene group from the para or meta position of SAHA's phenyl group represented by formula (IV):

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- 45 -

(IV)

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(2) attaching a 2-3 methyl linker followed by a phenyl or naphthalene group from the meta position of TSA's phenyl cap group, or from TSA's dimethyl amino group represented by formula (V):

(V)

phenyl or napthalene

phenyl or napthalene

n(H₂C)

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and which may bind in groove B is a 1-3 methyl group spacer followed by a carboxylate, sulfate or phenyl group as represented by formula (VI):

(VI)

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With respect to the aliphatic (Y) group, the diameter of the pocket suggests that one more methyl "side chain" could fit, in addition to the C15 methyl group on the C10 carbon. Nonlimiting suitable examples for Y constituents wherein Y comprises an aliphatic chain group are as follows: (1) add

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a methyl group to TSA on the C12 carbon (with or without a methyl group on the C10 carbon and with or without double bonds and with or without substituting the X and/or Z constituents of formula (I)as represented by formula (VII):

(VII)

10 (2) add a methyl group to TSA on the C9 carbon (with or without a methyl group on the C10 carbon; with or without both or either of the double bonds, and with or without substituting the X and/or Z constituents of formula (I) as represented by formula (VIII):

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(VIII)

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(3) replace the two alkalene double bonds of TSA with only one between C10 and C11, which may free the C11 and C12 torsion to allow for a better fit, the X and/or Z groups may also be substituted as represented by formula (IX):

25 (IX)

(4) cyclize C15 and C12 carbons of TSA through a sulphur atom (or nitrogen atom), the X and/or Z groups may also be substituted as represented by formula (X):

(X)

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(5) extend from the C9 carbon of TSA such that the extension approaches and/or enters groove B (see Figure 9); making C9 sp3 so that it can have some freedom; attach to C9 a 1-3 methyl group spacer which may include a double bond and they attaching thereto a sulfate, carboxylate, sulfate, hyroxyl, or phenyl group which may make an interaction with the N-epsilon proton of His170 which may coordinate the zinc atom as represented by formula (XI):

(XI)

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$$X \longrightarrow \begin{pmatrix} (1s) & ($$

25 (6) extend off the C8 carbon (replacing C14) of TSA such that the extension approaches or enters groove B; attach a 1-3 methyl group spacer (which may include a double bond) and then link thereto a carboxylate, sulfate, hydroxyl or phenyl group such that an interaction is made with the N-epsilon proton of His170 that coordinates the zinc atom; the X and/or Z constituents may also be substituted as represented by formula (XII):

- 48 -

(XII)

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&$$

(7) substitute the C8 carbon at the end of the aliphatic chain such that the substitution may contact groove A, A', B and or C, in such an example, a cap group (X) may or may not be required and the X and Z constituents may be substituted as well, as represented by formula (XIII):

(XIII)

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(8) formulas VII through XIII above wherein the aliphatic chain further comprises a methyl group between the active site binding group (Z) and the C8 carbon, and preferably just before the C8 carbon, increasing the distance between X and Z, (9) make the connection between the aliphatic chain and the cap group more rigid (e.g., by closing a 6-membered ring which may or may not comprise oxygen, the X and Z group may also be substituted as represented by formula (XIV):

(XIV)

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and (10) combining two or more of the changes depicted by formulas (VII-XIV).

Additionally, nonlimiting examples for suitable Z groups wherein Z comprises an active site binding group are as follows: (1) hydroxamic acid, (2) carboxylic acid, (3) sulfonamide, (4) acetamide, (5) epoxyketone, (6) an ester with a methyl linker and a hydroxyl of acetate ester group to lead into the cavity and interact with a conserved arginine (Arg27) as represented by formula (XV): (XV)

$$R_1 = \begin{cases} CH_2 \text{ in } \\ C \\ C \\ C \\ C \end{cases}$$

$$R_1 = \begin{cases} -OH \\ -C \\ O - CH_3 \end{cases}$$

and (7) an alphaketone as represented by formula (XVI):

$$R_{1} = \begin{cases} --- (CH_{2})n - OH \\ --- (CH_{2})n - CH_{2} \end{cases}$$

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Additionally, other suitable X, Y and Z constituents may be envisioned by the skilled artisan given the three-dimensional structural information of the present invention.

After having determined potential suitable X, Y and Z constituents, the constituents are combined to form a compound of formula (I) using combinatorial chemistry techniques. This may be achieved according to U.S. Patent Nos. 5,608,108; 5,700,811; 5,773,474; 5,840,960 and 5,668,179, incorporated herein by reference. Any methods

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known to one of skill in the art may be employed to synthesize compounds of formula (I) comprising X, Y and Z constituents as determined by the methods described above.

As mentioned above, the compounds of formula (I) are useful to inhibit the histone deacetylase activity of HDLP and HDAC-related proteins. Such inhibition may allow for a reduction or cessation of cell growth in vitro and in vivo.

For in vitro use, such reduction or cessation of cell growth is useful to study the role of histone deacetylation and differentiation during the cell cycle and also to study other mechanisms associated with cell cycle arrest and particularly how the repression of transcription is involved in cell cycle progression which may be studies in a yeast model system such as that described by Kadosh & Struhl, 1998, Mol. Cell. Biol. 18:5121-5127. In vitro model systems which may be employed to study the effects of potential inhibitors on cell cycle progression and also tumor growth include those described by: Richon et al, 1998, Proc. Natl. Acad. Sci. USA 95:3003-3007; Yoshida et al., 1995, Bioessays 17:423-430; Kim et al., 1999, Oncogene 18:2461-2470; Richon et al., 1996, Proc. Natl. Acad. Sci. USA 93:5705-5708; and Yoshida et al., 1987, Cancer Res. 47:3688-3691.

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For in vivo use, such a reduction or cessation of cell growth is useful to study the effect of said inhibitor compounds in non-human animal model systems of cancer and is also useful for the treatment of cancer in a recipient in need of such treatment. Non-limiting examples of animals which may serve as non-human animal model systems include

mice, rats, rabbits, chickens, sheep, goats, cows, pigs, and non-human primates. See, e.g., Desai et al., 1999, Proc. AACR 40: abstract #2396; Cohen et al., 1999, Cancer Res., submitted. The compounds of the present invention may be administered to a transgenic non-human animal wherein said animal has developed cancer such as those animal models in which the animal has a propensity for developing cancer (e.g. animal model systems described in U.S. Patents 5,777,193, 5,811,634, 5,709,844, 5,698,764, and 5,550,316). Such animal model systems may allow for the determination of toxicity and tumor reduction effectiveness of the compounds of the present invention.

A preferred compound of the present invention may comprise high specific activity for HDLP and HDAC-related proteins, good bioavailability when administered orally, activity in reducing or ceasing cell growth in tumor cell lines, and activity in reducing or ceasing tumor growth in animal models of various cancers.

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Accordingly, another aspect of this invention is a method of eradicating or managing cancer in a recipient, which may be an animal and is preferably a human. Said method comprises administering to said recipient a tumor reducing amount of a compound as defined by formula (I) above, or a physiological acceptable salt thereof.

In a further aspect of the invention, there is provided a composition comprising the compound of formula (I) and an excipient or carrier. Administration of the foregoing agents may be local or systemic. Such carriers include any

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suitable physiological solutions or dispersant or the like. The physiologic solutions include any acceptable solution or dispersion media, such as saline, or buffered saline. carrier may also include antibacterial and antifungal agents, isotonic and absorption delaying agents, and the like. Except insofar as any conventional media, carrier or agent is incompatible with the active ingredient, its use in the compositions is contemplated.

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- 10 Routes of administration for the compositions containing the delivery vehicle constructs of the present invention include any conventional and physiologically acceptable routes, such as, for example, oral, pulmonary, parenteral (intramuscular, intraperitoneal, intravenous (IV) or subcutaneous injection), inhalation (via a fine powder formulation or a 15 fine mist), transdermal, nasal, vaginal, rectal, or sublingual routes of administration and can be formulated in dosage forms appropriate for each route of administration.
- 20 The following examples are provided to more clearly illustrate the aspects of the invention and are not intended to limit the scope of the invention.

EXAMPLES

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Example 1: Protein Production and Purification: 25

Full-length wild-type HDLP (Genbank accession number AE000719) was subcloned from an Aquifex aeolicus chromosomal DNA preparation (provided by Robert Huber of Universitaet of Regensburg, Germany) into the pGEX4T3 (Amersham-Pharmacia, Piscataway, NJ) vector using the polymerase chain reaction The cysteine-to-serine and active site mutants were constructed by PCR site directed mutagenesis and were

sequenced. The HDLP-glutathione S-transferase (GST) fusion protein was produced in Escherichia coli, purified by chromatography using a column affinity glutathione-sepharose resin (Amersham-Pharmacia, Piscataway, NJ), and by anion-exchange chromatography (Q-sepharose™; Amersham-Pharmacia, Piscataway, NJ). HDLP was cleaved from the fusion protein with thrombin at 4°C, was purified by (Q-sepharose™; Amersham-Pharmacia, anion-exchange Piscataway, NJ) and qel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ), and was concentrated to typically 25 mg/ml in a buffer of 25 mM bis-tris propane (BTP), 500 mM NaCl, 5 mM dithiothrietiol (DTT), 2% isopropanol, pH 7.0.

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15 Although, it is not known what metal cofactor HDLP contains in vivo, it is presumed to be zinc because of arrangement of the ligands and the similarities in the active site to the zinc proteases. The lack of metal in the purified HDLP is presumed due, in part, to the use of DTT during purification. \mbox{HDLP} was reconstituted with \mbox{Zn}^{2+} by 20 mixing the Cys75Ser/Cys77Ser double mutant at 10 mg/ml with a 5-fold molar excess of ZnCl2 in a buffer of 25 mM bis-tris propane, 200 mM NaCl, 1% isopropanol, pH 7.0. Unbound ZnCl² was removed by fractionating HDLP through a G25 desalting 25 column (Amersham-Pharmacia, Piscataway, NJ). The HDLP-Zn²⁺-TSA complex was prepared by incubating the Zn²⁺ reconstituted HDLP mutant with 1 mM TSA for 45 minutes, followed by gel filtration chromatography (Superdex™200; Amersham-Pharmacia, Piscataway, NJ) to remove excess TSA, and concentration to typically 25 mg/ml in a buffer of 25 mM 30 bis-tris propane, 500 mM NaCl, 1% isopropanol, pH 7.0.

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FLAG epitope tagged human HDAC1 was overexpressed using a baculovirus expression system in Hi5 (Invitrogen, Carlsbad, CA) insect cells grown in suspension in serum-free media (Sf900, Gibco, Grand Island, NY). The fusion protein was purified by anion exchange and affinity chromatography using Anti-FLAG M2 affinity resin (Sigma, St. Louis, MO) and FLAG Peptide (Sigma, St. Louis, MO).

Example 2: Crystallization and data collection:

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10 Crystals of apo-HDLP were grown at room temperature by the hanging-drop vapor-diffusion method, from 7.5% isopropanol, 28% PEG 1500, 425 mM NaCl, 100 mM Tris-Cl, pH 7.0. They form in space group C2 with a = 51.4 Å, b = 93.8 Å, c = 78.7 Å, β = 96.9 Å, and contain one HDLP molecule in the asymmetric unit. Diffraction data were collected with crystals flash-frozen in a buffer of 7.5% isopropanol, 35% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, at -170° C.

The structure of the HDLP- $\rm Zn^{2+}$ complex was determined from HDLP Cys75Ser/Cys77Ser double mutant crystals grown from 23% tert-butanol, 27% PEG 1500, 400 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8. Space group and cell dimensions were identical to the apocrystals. The HDLP- $\rm Zn^{2+}$ crystals were harvested and frozen in 27% tert-butanol, 22% PEG 1500, 50 mM KCl, 20 mM NaCl, 0.2 mM ZnCl₂, 100 mM bis-tris propane, pH 6.8, at -170° C.

Crystals of the HDLP-Zn²⁺-TSA complex comprised HDLP Cys75Ser/Cys77Ser double mutant and were grown from 23% tert-butanol, 27% PEG 1500, 600 mM KCl, 100 mM bis-tris propane-Cl, pH 6.8, by microseeding. The crystals were grown in the presence of zinc. They form in space group

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 $P2_12_12_1$ with a = 53.4 Å, b = 94.4 Å, c = 156.3 Å and contain two HDLP- Zn^{2+} -TSA complexes in the asymmetric unit. The HDLP- Zn^{2+} -TSA crystals were harvested and frozen in the same cryobuffer as the HDLP- Zn^{2+} crystals except that 0.5mM TSA was added. Data were processed with DENZO and SCALEPACK (Otwinowski & Minor, 1997, Method. Ensemble. 276:307-326). MIR analysis, model building and refinement.

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The HDLP-Zn²⁺-SAHA complex crystals were grown and evaluated the same as the HDLP-Zn²⁺-TSA crystals. However, the restraints for the SAHA structure were constructed based on stereochemical parameters from TSA. Like the apo-HDLP crystals, the SAHA/HDLP co-crystals grew in space group C2.

Heavy-atom soaks were performed with the apo-HDLP crystals 15 in a buffer of 7.5% isopropanol, 30% PEG 1500, 75 mM NaCl, 100 mM Tris-Cl, pH 8.0, supplemented with 1.0 mM thimerosal for 2h, 5 mM KAu(CN)₂ for 1h, and 1 mM Pb(Me)₃OAc for 2h. MIR phases were calculated with the program MLPHARE (The 20 CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D 50:760-763) at 2.5 Å using the anomalous diffraction signal from the thimerosal derivative, and had a mean figure of merit of 0.55. The phases were improved by solvent flattening with the program DM (The CCP4 25 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D 50:760-763) , and were used to build the initial model with the program O (Jones et al., 1991, Acta Crystallogr. A 47:110-109). Successive rounds of rebuilding and simulated annealing refinement with the 30 program CNS (Brunger et al., 1998, Acta Crystallogr. D 54:905-921) allowed interpretation of HDLP from residues 2

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to 373. Residues 1, 374, and 375 were not modeled and are presumed to be disordered.

The structure of the HDLP-Zn2+-TSA and HDLP-Zn2+-SAHA complex were determined by molecular replacement with the program AMORE (The CCP4 suite: Programs for computational crystallography, 1994, Acta Crystallogr. D 50:760-763) using the apo-HDLP structure as a search model. The initial electron density maps had strong and continuous difference density for the entire TSA molecule. However the SAHA molecule was not as well ordered in the cap group region. The structure of TSA was obtained from the Cambridge Structural Database (Refcode TRCHST) and was used to define stereochemical restraints used in the refinement with the program CNS. The restraints of SAHA were constructed based on stereochemical parameters from TSA and surrounding amino acid residues. The dimer interface in the HDLP-Zn2+-TSA and HDLP-Zn²⁺-SAHA crystals primarily involves Phe200 on the protein surface. The Phe200 side chain contacts Tyr91, whose side chain conformation changes on TSA binding, and part of the dimethyl amino phenyl group of TSA from the second protomer. The HDAC family does not contain a phenylalanine residue at the equivalent position.

25 Example 3: Histone deacetylase assays:

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Purified proteins were assayed by incubating 10 μg of [3H] acetyl-labeled murine erythroleukemia histone substrate and HDAC assay buffer (20 mM Tris-HCl, pH 8.0, 150 mM NaCl, 10% glycerol) for 30-60 minutes at 37° C in a total volume of 30 μ l. The final concentrations of HDLP and HDAC1-FLAG were 3.6 μ M and 0.24 μ M, respectively. Assays were performed in duplicate. The reactions were stopped and the

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released acetate was extracted and assayed as described (Hendzel et al., 1991, J. Biol. Chem. 266:21936-21942). [3H] acetyl-labeled murine erythroleukemia histones were prepared essentially as described (Carmen et al., 1996, J. Biol. Chem. 271:15837-15844). Inhibitors were added in the absence of substrate and incubated on ice for 20 minutes, substrate was added, and the assay performed as described above. HDLP was inclubated with 20 μ M ZnCl₂ and 20 μ M MnCl₂(H2O)₄ in HDAC buffer and tested for activity.

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Only HDLP dialyzed against ${\rm ZnCl_2}$ had activity. HDAC1-FLAG was dialyzed against 20 μM ${\rm ZnCl_2}$ in HDAC buffer which had no effect on activity. Therefore, HDAC1-FLAG contains a metal as purified.

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The in vivo substrate of HDLP is not known. HDLP may have a role in acetoin utilization like the B. subtilis AcuC gene product, and it has been annotated as such in the genome sequence, but the reaction catalyzed by AcuC is also not known. Furthermore, the A. aeolicus genome appears to lack the acuA and acuB genes that are part of the acuABC operon of B. subtilis (Deckert et al., 1998 Nature 392:353-358), and HDLP is as similar to human HDAC1 (35.2 % identity) as it is to B. subtilis AcuC (34.7 % identity).

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What is claimed is:

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- 1. A crystal of an enzyme comprising deacetylase activity wherein said crystal effectively diffracts X-rays for the determination of the atomic coordinates of said enzyme to a resolution of greater than 4 Å and wherein the structure of said enzyme comprises a conserved core α/β structure characteristic fold wherein said conserved α/β fold comprises an eight-stranded parallel β sheet and eight α helices and wherein four of the helices pack on either face of said parallel β sheet and wherein said structure of said enzyme comprises an rmsd of less than or equal to 1.5 Å in the positions of α atoms for at least 2/3 or more of the amino acids of HDLP as defined by the atomic coordinates of HDLP.
- 2. The crystal of claim 1, wherein said protein structure further comprises:
 - (a) eight α helices positioned near one side of the β sheet; and
 - (b) at least seven large, well defined loops originating from the C-terminal ends of the β -strands of said eight-stranded parallel β sheet wherein the eight extra helices and the seven large loops are associated with a significant extension of the structure beyond the core α/β motif and wherein said extension of the structure gives rise to a deep, narrow pocket and an internal cavity adjacent to the pocket.

3. The crystal of claim 1, wherein said enzyme comprising deacetylase activity is selected from the group

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consisting of HDLP, HDLP-related proteins, HDAC1, HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, AcuC, and functional derivatives thereof.

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- 4. The crystal of claim 2 further comprising a specifically bound zinc atom in the active site of said enzyme.
- 10 5. The crystal of claim 2 further comprising a specifically bound deacetylase inhibitor compound in the active site of said enzyme.
- 6. The crystal of claim 2 define by the atomic coordinates according to Figure 16.
 - 7. A method for identifying a potential deacetylase inhibitor compound for an enzyme which comprises deacetylase activity, said method comprising the steps of:
 - using a three-dimensional structure of HDLP as defined by atomic coordinates according to Figure 16;
 - employing said three-dimensional structure to design or select said potential inhibitor;
 - c. synthesizing said potential inhibitor;
 - d. contacting said potential inhibitor with said enzyme in the presence of an acetylated substrate; and
- e. determining the deacetylase inhibitory activity of said potential inhibitor.

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8. The method of claim 7, wherein the three-dimensional structure is designed or selected using computer modeling.

- 5 9. The method of claim 7, wherein the potential deacetylase inhibitor is designed de novo.
 - 10. The method of claim 7, wherein the potential deacetylase inhibitor is designed based on a known inhibitor.

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- The method of claim 7, wherein said enzyme comprising deacetylase activity is selected from the group consisting of HDLP, HDLP-related proteins, HDAC1,
 HDAC2, HDAC3, HDAC4, HDAC5, HDAC6, HDAC-related proteins, APAH, and AcuC.
 - 12. A method of evaluating the binding properties of the potential deacetylase inhibitor compound comprising the steps of:
 - a. co-crystallizing said compound with HDLP;
 - b. determining the three-dimensional structure of said HDLP-potential inhibitor complex co-crystal by molecular replacement using the threedimensional structure of HDLP as defined by atomic coordinates according to Figure 16; and
 - c. analyzing said three-dimensional structure of said HDLP bound to said potential inhibitor compound to evaluate the binding characteristics of said potential inhibitor compound.
 - 13. A method for solving the structure of an HDAC family

member crystal comprising the steps of:

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- a. collecting X-ray diffraction data of said crystal wherein said data diffracts to a high resolution limit of greater than 4 Å;
- b. using the atomic coordinates of HDLP accoding to Figure 16 to perform molecular replacement or refinement and difference fourier with said X-ray diffraction data of said HDAC family member crystal to determine the structure of said HDAC family member; and
- c. refining said structure of said HDAC family member.
- 14. The method of claim 13, wherein said HDAC family member is HDAC1.
 - 15. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant is encoded by the nucleic acid sequence of SEQ ID NO:4.
 - 16. A Cys75Ser/Cys77Ser double mutant of HDLP wherein said mutant has the amino acid sequence of SEQ ID NO:3.
 - 17. A nucleotide sequence according to SEQ ID NO:4
 - 18. An expression vector comprising the nucleotide sequence of claim 17.
- 19. A method of using the crystal of claim 1 for screening for a novel drug comprising:
 - a. selecting a potential ligand by performing

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rational drug design with the three-dimensional structure determined for the crystal;

- b. contacting the potential ligand with the ligand binding domain of the crystal; and
- c. detecting the binding potential of the potential ligand for the ligand binding domain, wherein the novel drug is selected based on its having a greater affinity for the ligand binding domain than that of a known drug.

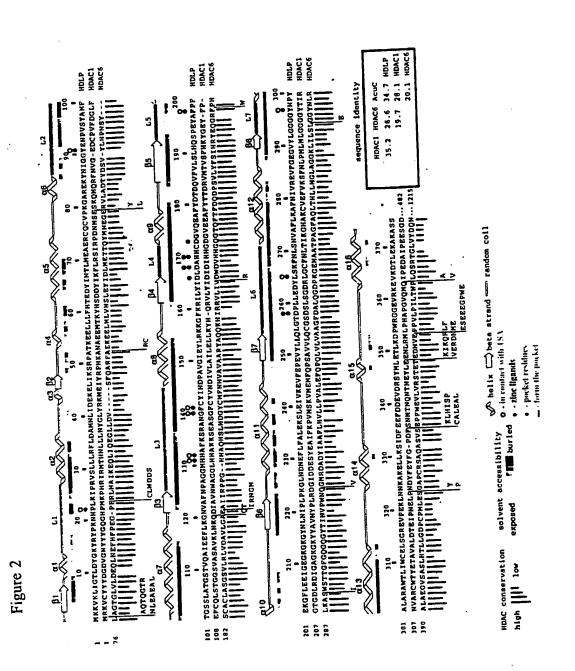
TABLE 1. Statistics from the crystallographic analysis

| | Nati | Native thi | thimerosal | g Q | Aucn | Zu | LSA | |
|-------------------------------|-------------|------------|------------|--------|--------|---------|---------|----------|
| Space Group Resolution (A) | C C 5 | | C2 2 8 | C 22 | C 8 | C 5 | P2,2,2, | |
| ons | 134.9 | | 79.023 | 11.454 | 27.722 | 125.769 | 180.427 | |
| flections | 32,1 | | 15,958 | 4.040 | 8.753 | 23.643 | 50.796 | |
| rage (%) | 92. | | 95.7 | 86.4 | 94.3 | 90.6 | 93.8 | |
| R _{sym} (%) | 2.5 | | 8.4 | 9.6 | 8.9 | 7.2 | 7.1 | |
| MIR analysis (20.0-2.5 Å) | <i>:</i> | | | | | | | |
| power | | | 1.47 | 1.24 | 1.10 | • | • | |
| | • | | 0.72 | 0.78 | 0.85 | • | | |
| Rcullis (ano) | | | 0.92 | • | | | | |
| Refinement statistics: | | | | | | | RMSD | |
| Resolution | Reflections | Total | Water | | | ponds | andles | B-factor |
| (Å) | | atoms | •• | | | (Å) | (C) | (A^2) |
| 4.8 | | 3214 | | 19.8 | 24.0 | 0.010 | 1.63 | 3.55 |
| HDLP-Zn 2.0 | 23,582 | 3424 | 434 | 22.0 | | 0.00 | 1.48 | 1.04 |
| HDLP-Zn-TSA 2.1 | 44.122 | 6475 | 456 | 22.4 | | 8000 | 1 78 | 3 83 |

merit = IF(hkl)best[/F(hkl). R-free = R-factor calculated using 5% of the reflection data chosen randomly and omitted from the start of refinement. RMSD: root mean square deviations from ideal geometry and root $\mathsf{F}_{\mathsf{calc}}$ $|\Sigma|_{\mathsf{obs}}$, where $\mathsf{F}_{\mathsf{obs}}$ and $\mathsf{F}_{\mathsf{calc}}$ are the observed and calculated structure factors, respectively. Figure of Asym = $\Sigma_h\Sigma_i$ (h,i-<h/>t/sh\inline | h,i for the intensity (I) of i observations of reflection h. Phasing power = <F_{\(\mu \> \)}/E, where <F₁1>is the root-mean-square heavy atom structure factor and E is the residual lack of closure error. Rcullis is the mean residual lack of closure error divided by the dispersive difference. R-factor $= \Sigma l F_{obs}$ mean square variation in the B-factor of bonded atoms.

Figure 1

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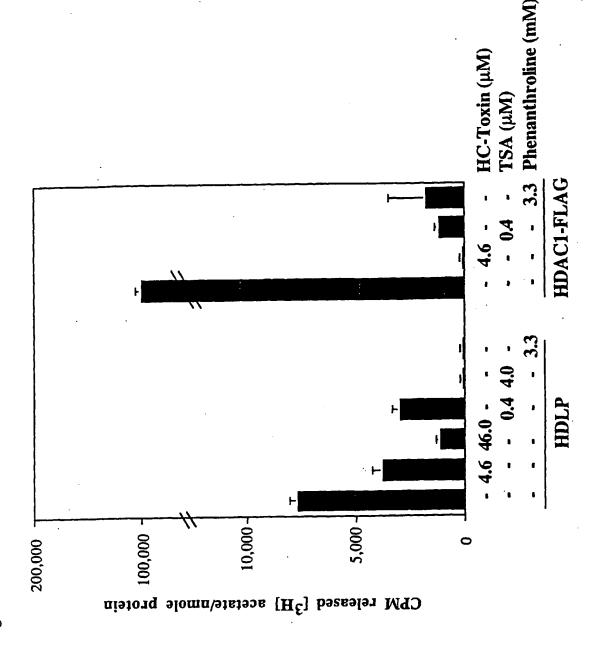
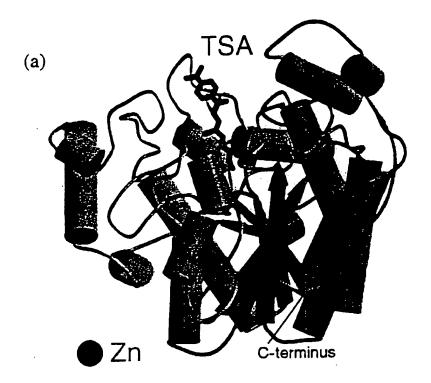


Figure 3

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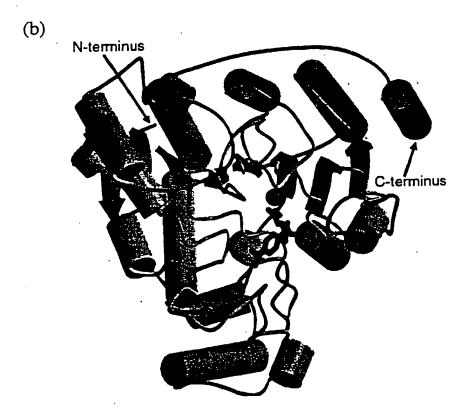
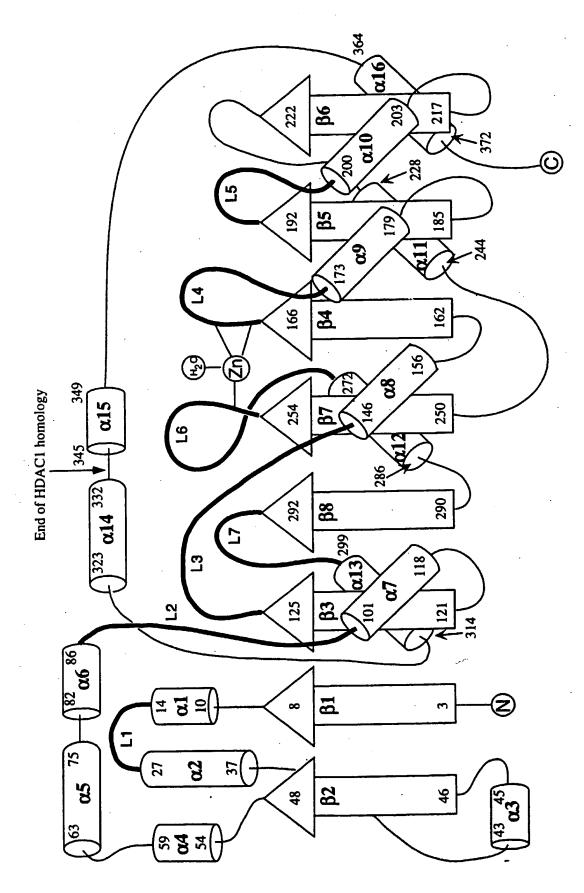
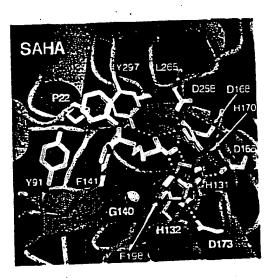


Figure 4



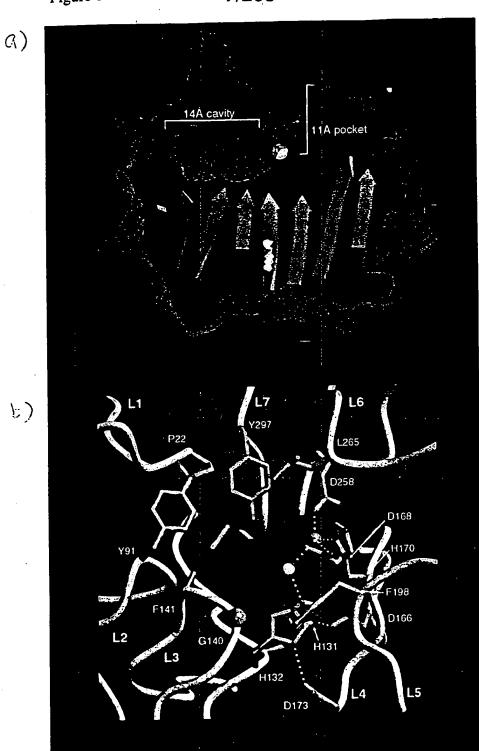
igure 40



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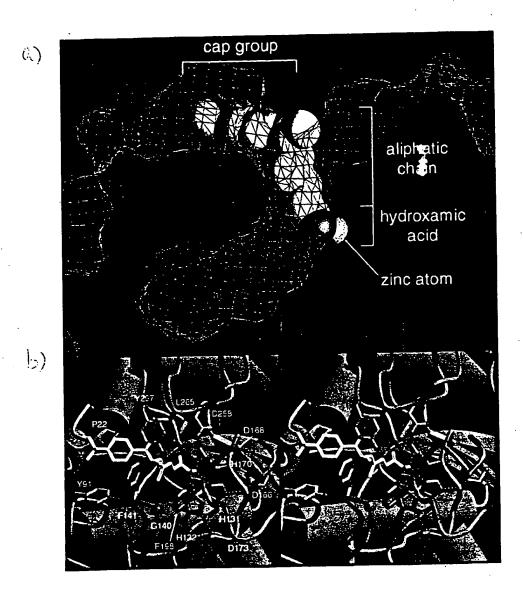
Figure 5

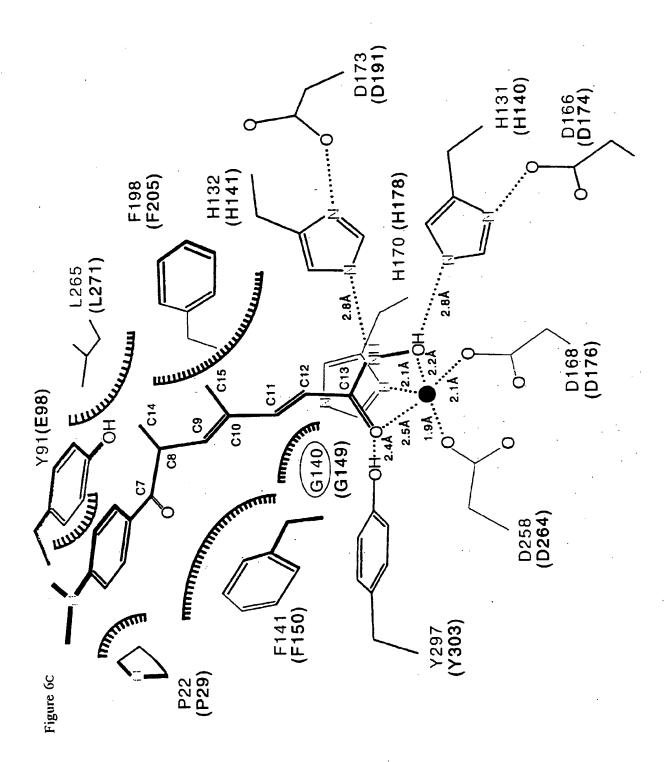
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Figure 6

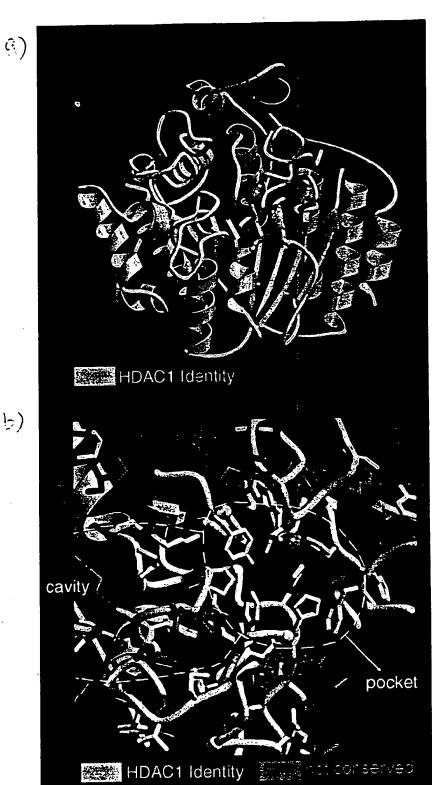




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Figure 7



b)

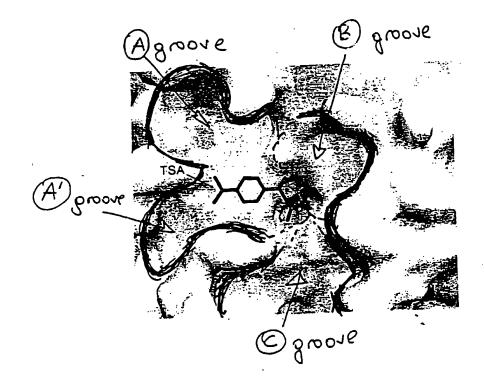


Figure 9

| 10 | 20 | 30 | 40 |
|---|----------------|---------------|-------------|
| سلسلس | ستلسب | سيلس | لسبل |
| ATGAAGAAGGITA | AACTTATCGGA | ACTITAGACTI | ACGGAA 40 |
| AGTACAGATATCC | CAAAAACCATC | CICTTAAAAT | ACCAAG 80 |
| AGTITCCCTACTC | | | |
| ATAGATGAGAAGG | AATTAATCAAG | AGCAGACCCG | CAACTA 160 |
| AAGAAGAACTCCT | | | |
| 210 | 220 | 230 | 240 |
| سلسسس | | | |
| CACTITAATGGAA | CCGGAAAGGIG | TCAGIGCGIT | CCGAAG 240 |
| GGAGCTAGGGAAA | | | |
| CCGTATCTTACCC | GATGITTACAG | GCICITCICI | CGCAAC 320 |
| GGGTTCAACAGTC | | | |
| AATGTAGCTTICA | LATCCCGCGGGA | GGTATGCACC | ACCCTT 400 |
| 410 | 420 | 430 | 44 0 |
| سيليبين | سيلسين | سيلينيا | |
| TTAAAAGCAGGG | CAAACGGCTTTT | GCTACATAAA | CGACCC 440 |
| CCTCTCCCAAT | GAGTACTIGAG | ;AAAAAAAAGGC | TTTAAG 480 |
| AGAATACICTAC | TAGACCITGAT | GCCCACCACT | GCGACG 520 |
| GIGITCAGGAAG | | | |
| CCIGICCCITCAC | | | |
| 610 | 620 | 630 | 640 |
| <u></u> | سيليييل | <u> </u> | 11111 |
| GAGAAGGGCTTC | TIGGAGGAGATA | AGGAGAAGGAA | AAGGAA 640 |
| AGGGCTACAACC | IGAACATTCCCC | TIGCCAAAGGC | CTIGAA 680 |
| CGACAACGAGTT | CICITIGCCCI | 'AGAAAAATC'I | CIGGAA 720 |
| ATAGICAAAGAA | FIATITGAGCCC | GAGGITTACC | TICITC 760 |
| AACTCGGAACTG | ACCCACICCITO | AAGATTACCI | TICCAA 800 |
| 810 | 820 | 830 | 840 |
| بيلينيانين | سيلسيان | سيلبين | لبييل |
| GITCAACCICIC | AAACGTTGCCTT | TTTAAAAGC: | MTCAAC 840 |
| ATCGITCGIGAG | GTTTTCGGGGA | GGAGTATAC | CTCGGAG 880 |
| GAGGCGGATACC | | | |
| CCTAATCTCGTG | | | |
| AAGCTAAACAAT | | | |
| 1010 | 1020 | 1030 | 1040 |
| <u></u> | | | |
| ACTITGAAGAGI | | | |
| ACTITICAACAST CCTCGAAACCCT | | | |
| ACGAAAGAAGTA | | | |
| CATCTIA 1127 | - TINITALING I | - Characacaca | |
| , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | | |

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| | 10 | 20 | 30 | 40 | |
|------------------|-----------|-----------|---------------------------|---------|-----|
| بيليين | لتستليد | سسلس | ستلسب | لسبيل | |
| MKKVKLI | GTLDYGKY | RYPKNHPLK | IPRVSLLLRE | LDAMNL | 40 |
| IDEKELI | KSRPATKE | ELLLFHTED | YINTIMEAET | RCQCVPK | 80 |
| GAREKYN | IIGGYENPV | SYAMFIGSS | LATGSTVQA | CEEFLKG | 150 |
| NVAFNPA | GGMHHAFK | SRANGFCYI | NDPAVGIEYI | LRKKGFK | 160 |
| RILYIDL | DAHHCDGV | QEAFYDIDQ | VFVLSLHQSI | PEYAFPF | 200 |
| | 210 | 220 | 230 | 240 |) . |
| سلست | لينتثلث | سيلس | Ludu | لسبيل | |
| EKGFLEE | IGEGKGKG | YNLNIPLPK | GLNDNEFLFA | ALEKSLE | 240 |
| די זוצויה זוניים | | | | | |
| TAVEALE | PEVYLLQL | GIDPLLEDY | LSKFNLSNV | YFLKAFN | 280 |
| | _ | | LSKFNLSNV7 AWI'LIWCELS | | |
| IVREVFG | EGVYLGGG | GYHPYALAR | | GREVPE | |

| | 10 | 20 | 30 | 40 |
|-----------|-------------------|-------------------|------------------|--|
| سلسد | سلسبان | بيلينينين | سلسسلت | سلت |
| ATGAAGA | AGGTTAAACT | TATOGGAACT | TTAGACTACG | GAA 40 |
| AGTACAG! | TATCCCAAA | AACCATCCTC | TTAAAATACC | AAG 80 |
| AGITTCCC | TACTCCITA | GGTTTTTAGA | TGCCATGAAC | CTT 120 |
| ATAGATGA | AGAAGGAATT. | AATCAAGAGC | 'AGACCCGCAAI | CTA 160 |
| AAGAAGAZ | ACTCCTTTTA' | TTCCACACGG | AAGACTACAT | AAA 200 |
| | 210 | 220 | 230 | 240 |
| سلسب | | | سلسيليد | |
| | | | GIGOGITOCG | |
| | | | GGATACGAAA | |
| | | | CITCICICGC | - |
| GGGTTCAF | CAGTGCAGG | CGATAGAGGA | SAATTITTA | 3GA 360 |
| AATGTAG | TTTCAATCC | CGCGGGAGGT | 'ATGCACCACG | CIT 400 |
| | 410 | 420 | 430 | 440 |
| سلسب | ىىلىسىلى <u>.</u> | <u></u> | ببليبيليد | ــــــــــــــــــــــــــــــــــــــ |
| TTAAAAGC | AGGGCAAAC | ECTITICET | 'ACATAAACGA(| CCC 440 |
| | | | AAAAGGCTTT | |
| AGAATACI | CTACATAGA | CTTGATGCC | CACCACTGCG | ACG 520 |
| GIGITCAC | GAAGCCTTT. | PACGATACAG | ACCAGGIGIIN | CGT 560 |
| CCTGTCCC | TTCACCAGI | CCCCGAGTA | CCCTTTCCC | TTT 600 |
| | 610 | 620 | 630 | 640 |
| سلسد | بيلينيان | ببليبيان | سلسسلت | ا ألب |
| GAGAAGGG | CITCCIGGAC | GAGATAGGA | GAAGGAAAAG | GAA 640 |
| AGGGCTAC | AACCIGAACA | ATTCCCCTGC | CAAAGGGCTT | 3AA 680 |
| CGACAACG | AGITCCICIT | PTGCCCTAGA | AAAATCTCTG | GAA 720 |
| ATAGICAA | AGAAGTATT | TGAGCCCGAG | GITTACCITC: | MC 760 |
| AACTCGGA | ACTGACCCAC | CICCIIGAAG | ATTACCTTTC | 008 AA |
| ç | 310 | 820 | 830 | 840 |
| _ | - | | | |
| GITCAACT | יייראאארניזיי | <u>مربینینینی</u> | AAAGCTTTCA | AC 840 |
| | | | TATACCTCGG | |
| | | | AAGGGCATGG | |
| | _ | | GAAGTGCCGG | |
| • | | • | TAAAGAGTAT | |
| | | | | |
| | | U2U . | | .1 |
| | | | CCCTCGTAC | ATT 1040 |
| | | | GGAGGAGAGG | |
| | | | AGGCGAAAGC | |
| CATCITA 1 | | | | - - |
| ~ ~ ~ T | ا مهد | | | |

| | 10 | 20 | 30 | 40 | |
|---------|----------|------------|------------|---------|-----|
| سلسب | لبسلير | سيبليين | <u> </u> | ليتيل | |
| MKKVKLI | GTLDYGK | RYPKNHPLK | IPRVSLLLR | FLDAMNL | 40 |
| | | | YINTLMEAE | | |
| | | | LATGSTVQA | | |
| | | | NDPAVGIEY | | 160 |
| | | | VFVLSLHQS | | 200 |
| | 210 | 220 | 230 | 240 |) |
| بيليين | سبيلي | سيطينيا | سلسند | لسبيل | |
| EKGFLEE | TGEGKGK | GYNLNIPLPK | GLNDNEFLF | ALEKSLE | 240 |
| IVKEVFE | PEVYLLQI | GTDPLLEDY | LSKFNLSNV | AFLKAFN | 280 |
| | | | RAWILIWCEL | | 320 |
| KLNNKA | | | | | 360 |
| | | | | | ••• |

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| | 10 | 20 | 30 | 40 |
|----------|------------------|------------------|--------------------------|-----------------|
| بيليين | uluul | uduul | سلسسلس | لبب |
| ATGAAGA | AGGITAAACI | TATOGGAAC | TTTAGACTAC | GAA 40 |
| AGTACAG | ATATCCCAA | AACCATCCI | CTTAAAATAC | CAAG 80 |
| AGTTTCC | CTACTCCTTA | GTTTTAG | ATGCCATGAAC | CTT 120 |
| ATAGATG | AGAAGGAATT | TAATCAAGAG | CAGACCCGCAZ | CTA 160 |
| AAGAAGA | ACTOCTTTT | YTTCCACACG | GAAGACTACAT | AAA 200 |
| | 210 | 220 | 230 | 240 |
| سلست | ببليستليد | بلبيتليد | بالسيالية | لب |
| CACTTTA | ATGGAAGCGG | AAAGGAGIC | AGAGCGTTCCC | AAG 240 |
| GGAGCTA | GGGAAAAGTA | CAACATAGG | COGATACGAAA | ACC 280 |
| CCGTATC | TTACGCGATG | TTTACAGGC | Terrereres | 'AAC 320 |
| GGGTTCA | ACAGTGCAGG | CGATAGAGG | AATTTTTAA | XXXX 360 |
| AATGTAG | CTTTCAATCC | CGCGGGAGG | TATGCACCACC | CTT 400 |
| | 410 | 420 | 430 | 44 0 |
| ببليب | سليسلب | بلينييان | بالتسليب | لبب |
| CAAAATT | CAGGGCAAAC | GCTTTTGC | TACATAAACGA | CCC 440 |
| CCCICIC | GAATTGAGT. | ACTIGAGAA | AAAAAGGCTTT | 'AAG 480 |
| AGAATAC: | ICTACATAGA | CCTTGATGC | CACCACTGCG | ACG 520 |
| GIGIICA | GAAGCCTTT | TACGATACA | GACCAGGIGII | CGT 560 |
| CCIGICC | CITCACCAGI | CGCCCGAGT | ACGCCTTTCCC | TTT 600 |
| | 610 | 620 | 630 | 640 |
| سيلس | سلسسلت | بلنبيلي | سلسبلب | 41 |
| GAGAAGG | CTTCCTGGA(| GAGATAGG: | AGAAGGAAAAG | GAA 640 |
| AGGGCTAC | CAACCTGAAC | ATTOCCCTG | CAAAGGGCTT | GAA 680 |
| CGACAACC | SAGITCCICT | ITGCCCTAGA | AAAAATCTCTG | GAA 720 |
| ATAGICA | AGAAGTATT. | IGAGCCCGA(| GITTACCTTC | TTC 760 |
| AACTOGGA | ACTGACCCA(| CICCIIGAAC | CATTACCTTTC | CAA 800 |
| | 810 | 820 | 830 | 840 |
| ببيليين | <u></u> | | | |
| | | | PAAAAGCTTTC | |
| | | | AGTATACCTCO | |
| | | | CAAGGGCATG | |
| | | | GGAAGIGCCG | |
| | | | TTAAAGAGTA | |
| • | 1010 | 1020 | 1030 | 1040 |
| | | | <u> </u> | |
| | | | ACCGCTCGTA | |
| | | | accoctecta Accaccacac | |
| | | | AAGGCGAAAG | |
| AICITA | | | | |

Figure 15

| | 10 | 20 | 30 | 40 | 1 |
|---------|-----------------|-----------|------------|----------|-----|
| سلسس | ليبيلين | سيلس | ساسيد | | |
| MKKVKLI | GILDYGKY | RYPKNHPLK | IPRVSLLLRI | LIDAMNIL | 40 |
| IDEKELI | KSRPATKE | ELLLFHIED | YINTLMEAET | RSOSVPK | 80 |
| GAREKYN | IGGYENPV | SYAMFIGSS | LATGSTVQAI | EEFLKG | 120 |
| NVAFNPA | GCMHHAFK | SRANGFCYI | NDPAVGIEYI | RKKGFK | 160 |
| | | | VFVLSLHQSE | | |
| | 210 | 220 | 230 | 240 |) |
| سلسب | سنتبلب | سيلس | سيلسب | | , |
| | | | GLNDNEFLFA | | 240 |
| IVKEVFE | PEVYLLQLO | TOPLLEDY | SKFNLSNVA | FLKAFN | 280 |
| IVREVFG | EGNATGGG | YHPYALARA | WILIWCELS | GREVPE | 320 |
| | | | SYMLETLKOP | | |
| | EKAKASS | | | | |

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| | | | | | riguic ro | | | | |
|------|-----------|------|-----------------|----------------|-----------|---------|--------|--|--------------|
| | | | | Residue | | Y | 2 | OCC. B | Segment ID |
| ATOM | 1 | CB | ALA | 2 | 45.336 | 35.880 | TE.042 | 1.10 59.90 | ÄÄÄÄ |
| ATOM | 2 | С | غند | 2 | 46.410 | 38.631 | 73.629 | 1.00 52.57 | AAAA |
| ATOM | 3 | Ö | ALA | 2 | 45.780 | 39.595 | 74.052 | 1.00 62.46 | AAAA |
| | 4 | 31 | ALA | 2 | 47.540 | 37.826 | 75.673 | 1.00 58.52 | AAAA |
| ATOM | | Cà. | ALA | 2 | 46.568 | 37.432 | 74.527 | 1.00 57.32 | AAAA |
| ATOM | 5 | | | | 46.330 | 38.570 | -2.389 | 1.00 39:61 | AAAA |
| ATOM | 6 | N | _7S | 3 | | | | 1.35 19.58 | |
| ATOM | 7 | CA | .1YS | 3 | 46.527 | 39.669 | | 1.00 19.58 | AAAA |
| ATOM | 8 | C3 | LYS | 3 | 47.855 | 39.763 | 73.459 | 1.00 36.03 | , shhh |
| ATCM | 9 | CG | LYS | . 3 | 49.217 | 40.007 | 71.102 | 1.00 55.16 | AAAA. |
| ATOM | 10 | CD | 178 | 3 | 50.315 | 40.000 | 70.039 | 1.00 66.28 | AAAA |
| ATOM | 11 | CΞ | LYS | 3 . | 51.700 | 40.163 | 70.655 | 1.00 73.41 | àààà |
| | 12 | NZ | LYS | 3 | 52.791 | 40.047 | 69.642 | 1.00 69.64 | AAAA |
| ATOM | | | - 110 | 3 | 45.407 | 39.422 | 70.642 | 1.50 23.29 | AAAA |
| ATOM | 13 | C | LYS | | | 38.262 | -3.487 | 1.00 27.41 | AAAA' |
| ATOM | 14 | C | LYS | 3 | 44.984 | | | 1.30 15.18 | |
| ATOM | 15 | N | ::AL | 4 | 44.314 | 40.498 | 70.138 | 1.50 12.15 | AAAA |
| ATOM | 16 | CA | 7AL | 4 | 43.535 | 40.418 | 69.349 | 1.00 22.20 | AAAA |
| ATOM | 17 | CB | ∵aL | 4 | 42.501 | 41.365 | ≨9.887 | 1.00 31.46 | شككة |
| ATOM | 18 | CGl | \therefore AL | 4 | 41.214 | 41.202 | 69.066 | 1.00 26.55 | شششة |
| ATOM | 19 | CG2 | VAL | 4 | 42.244 | 41.080 | ~1.348 | 1.00 34.98 | AAAA. |
| ATOM | 20 | c | VAL | 4 | 43.983 | 40.851 | 67.961 | 1.00 15.33 | AAAA |
| ATOM | 21 | Ö | 7AL | 4 | 44.557 | 41.927 | 67.778 | 1.00 31.19 | AAAA |
| | | | LYS | 5 | 43.654 | 40.023 | 46.978 | 1.00 21.82 | AAAA |
| ATOM | 22 | N | | 5 | 44.052 | 40.291 | 65.607 | 1.00 10.10 | AAAA |
| ATOM | 23 | CA. | LYS | 3 | 44.722 | 40.252 | 25.507 | 1.20 23.35 | |
| ATOM | 24 | CB | LYS | 5 | 45.047 | .39.214 | 65.177 | 1.30 20.10 1.30 23.35 1.30 23.75 | AAAA |
| ATOM | 25 | CG | LYS | 5 | 46.301 | 39.092 | 55.049 | 1.10 13.75 | AAAA |
| ATOM | 26 | CD | LYS | 5 | 47.183 | 40.334 | 65.919 | 1.00 03.70 | AAAA |
| ATOM | 27 | CE | LYS | 5 | 48.510 | 40.151 | 55.669 | 1.30 04.34 | AAAA |
| ATOM | 28 | :12 | LïS | 5 | 49.351 | 41.387 | 66.585 | 1.10 11.04 | AAAA |
| ATOM | 29 | C | LYS | 5 | 42.914 | 40.294 | 64.596 | 1.30 00.27 | ääää |
| ATOM | 30 | Ö | LYS | 5 | 41.949 | 39.535 | 54.728 | | AAAA |
| ATOM | 31 | N | LEU | 6 | 43.071 | 41.111 | 53.564 | 1.00 19.28 | AAAA |
| | | CA | LEU | 6 | 42.097 | 41.156 | 52.483 | 1.00 20.68 | AAAA |
| atom | 32 | | LEU | 6 | 41.571 | 42.574 | 62.291 | 1.00 23.51 | ÀAAÀ |
| ATOM | 33 | CB | | | 40.373 | 42.712 | 51.342 | 1.00 30.59 | AAAA |
| atom | 34 | CS | LEU | 6 | | | | | AAAA |
| ATOM | 35 | | LEU | 6 | 40.079 | 44.192 | 51.153 | | |
| ATOM | 36 | 552 | LEU | 5 | 40.557 | 42.085 | 59.995 | 23.53 | aaaa |
| atom | 37 | Ξ | LEU | 6 | 42.954 | 40.701 | 51.237 | 1.00 19.17 | AAAA |
| ATOM | 38 | 0 | LEU | ő | 43.911 | 41.249 | 60.919 | 1.00 22.31 | AAAA |
| ATOM | 39 | :: | ILE | 7 | 42.359 | 39.689 | 50.538 | 1.30 19.15 | ሕሕሕ ሕ |
| ATOM | 40 | CA | ILE | 7 | 43.045 | 39.139 | 59.338 | 1.00 13.38 | ääää |
| ATOM | 41 | 23 | ILE | 7 | 42.922 | 37.674 | 59.191 | 1.00 19.05 | AAAA |
| ATOM | ÷2 | 132 | ILE. | ~ | 43.930 | 37.162 | 53.144 | 1.10 16.45 | AAAA |
| | ÷3 | 231 | ELE | - | 43.253 | 37.007 | 50.521 | 1.00 12.81 | inhin |
| ATOM | | | ILE | - | 43.296 | 35.543 | 50.450 | 1.00 34.99 | AAAA |
| ATOM | 14 | === | | . - | 42.396 | 39.850 | 58.125 | 1.00 17.95 | ÁÁÁÁ |
| ATOM | 45 | - | | | | | | 1.30 17.95 | AAAA |
| STOM | 46 | = | TLE | 7 | 41.138 | 39.729 | 57.928 | 1.00 17.70 | |
| ATOM | 47 | :: | GLY | 3 | 43.193 | 40.552 | 57.330 | | AAAA. |
| ATOM | 48 | ·CA | jĽY | 5 | 42.523 | 41.193 | 56.148 | 1.30 18.11 | AAAA |
| ATOM | 19 | 2 | 3LY | 3 | 43.640 | 41.957 | 55.243 | 1.00 10.91 | AAAA. |
| ATOM | 50 | 9 | GLY | 3 | 44.849 | 41.840 | 55.504 | 1.00 22.27 | AAAA. |
| ATOM | 51 | 21 | THR | 9 | 43.134 | 42.428 | 54.155 | 1.00 13.99 | ሕ ልሕሕ |
| ATOM | 52 | CA | THR | 9 | 43.950 | 43.141 | 53.183 | 1.00 25.95 | تهممن |
| | 53 | C3 | THR | 9 | 44.739 | 42.195 | 52.263 | 1.30 15.80 | AAAA |
| atom | | | | ۇ د | 45.321 | 42.962 | 31.199 | 1.30 25.56 | AAAA |
| ATOM | E 4 | 331 | THR | 2 | 43.823 | 41.144 | 51.657 | 1.30 25.56 | AAAA |
| ATOM | 55 | 237 | THR | 9 | | | | 1.00 29.04 | AAA. |
| atom | 56 | C32 | THR | è | 43.025 | 43.957 | 52.294 | 1.00 23.05 | |
| ATOM | 57 | :: | THR | 9 | 41.972 | 43.582 | 52.082 | 1.00 23.05 | AAAJ |
| ATCM | 56 | :: | LEU | 10 | 43.517 | 45.079 | ≣1.781 | 1.30 29.19 | AAA |
| ATCM | 59 | CA | LEU | 10 | 42.690 | 45.396 | 50.895 | 1.30 32.55 | iaaa |
| ATCM | 50 | 23 | LEU | 10 | 43.256 | 47.319 | 50.761 | 1.00 28.09 | AAAi |
| ATOM | 5i | 33 | LEU | 15 | 43.142 | 48.256 | 51.958 | 1.30 33.00 | AAA |
| | 62 | ==: | LEU | 10 | 41.580 | 48.403 | 52.347 | 1.00 26.65 | AAA |
| ATOM | | ==== | LEU | 10 | 43.938 | 47.744 | 53.126 | 1.00 41.33 | AAA |
| atom | 63 | | | 10 | 42.556 | 45.261 | 49.512 | 1.00 32.68 | AAA |
| atom | 64 | _ | LEU | | | 45.684 | 48.702 | 1.30 26.97 | AAA. |
| ATCM | 55 | Ξ | LEU | 10 | 41.736 | | | 1,30 25.75 | in his |
| ATOM | 56 | :: | ASP | 11 | 43.377 | 44.234 | 49.256 | _, | C-1747 |
| | | | | | | | - | | |

| ATOM | 67 | CA | ASP | 11 | 43.367 | 43.541 | 47.970 | 1.00 35.74 | AAAA |
|------|------|----------|-----|------|--------|--------|--------|------------|------|
| | 68 | CB | ASP | 11 | 44.477 | 42.485 | 47.922 | 1.00 37.61 | AAAA |
| ATOM | | | ASP | 11 | 45.858 | 43.093 | 48.079 | 1.00 46.75 | AAAA |
| MOTA | 69 | CG | | | | | | 1.00 46.34 | AAAA |
| ATOM | 70 | | ASP | 11 | 46.110 | 44.136 | 47.444 | | |
| ATOM | 71 | OD2 | ASP | 11 | 46.690 | 42.528 | 48.821 | 1.00 58.94 | AAAA |
| MOTA | 72 | С | ASP | 11 | 42.034 | 42.898 | 47.607 | 1.00 34.26 | AAAA |
| ATOM | 73 | 0 | ASP | 11 | 41.748 | 42.696 | 46.420 | 1.00 31.12 | AAAA |
| | 74 | N | TYR | 12 | 41.220 | 42.558 | 48.609 | 1.00 26.19 | AAAA |
| MOTA | | | | 12 | 39.923 | 41.963 | 48.314 | 1.00 28.45 | AAAA |
| MOTA | . 75 | CA | TYR | | | | | 1.00 29.35 | AAAA |
| MOTA | 76 | CB | TYR | 12 | 39.119 | 41.720 | 49.601 | | |
| MOTA | 77 | CG | TYR | 12 | 39.648 | 40.595 | 50.470 | 1.00 28.47 | AAAA |
| ATOM | 78 | CD1 | TYR | . 12 | 40.137 | 40.846 | 51.755 | 1.00 32.17 | AAAA |
| MOTA | 79 | CE1 | TYR | 12 | 40.592 | 39.808 | 52.572 | 1.00 30.35 | AAAA |
| | 80 | | TYR | 12 | 39.629 | 39.276 | 50.017 | 1.00 22.97 | AAAA |
| ATOM | | | TYR | 12 | 40.077 | 38.228 | 50.822 | 1.00 19.60 | AAAA |
| MOTA | 81 | | | 12 | 40.554 | 38.499 | 52.096 | 1.00 21.42 | AAAA |
| MOTA | 82 | CZ | TYR | | | | 52.907 | 1.00 23.49 | AAAA |
| MOTA | 83 | ОН | TYR | 12 | 40.964 | 37.456 | | | AAAA |
| ATOM | 84 | С | TYR | 12 | 39.144 | 42.907 | 47.390 | 1.00 26.67 | |
| MOTA | 85 | 0 | TYR | 12 | 38.307 | 42.466 | 46.593 | 1.00 30.51 | AAAA |
| ATOM | 86 | N | GLY | 13 | 39.441 | 44.201 | 47.492 | 1.00 30.22 | AAAA |
| ATOM | 87 | CA | GLY | 13 | 38.767 | 45.203 | 46.675 | 1.00 25.13 | AAAA |
| | 88 | C | GLY | 13 | 38.911 | 45.009 | 45.177 | 1.00 27.31 | AAAA |
| MOTA | | | GLY | 13 | 38.096 | 45.522 | 44.415 | 1.00 29.38 | AAAA |
| MOTA | 89 | 0 | | | 39.937 | 44.269 | 44.755 | 1.00 33.56 | AAAA |
| ATOM | 90 | N | LYS | 14 | | | | 1.00 39.81 | AAAA |
| MOTA | 91 | CA | LYS | 14 | 40.176 | 44.005 | 43.337 | _ | |
| MOTA | 92 | CB | LYS | 14 | 41.680 | 44.026 | 43.031 | 1.00 51.10 | AAAA |
| MOTA | 93 | CG | LYS | 14 | 42.292 | 45.424 | 42.907 | 1.00 64.99 | AAAA |
| MOTA | 94 | CD | LYS | 14 | 41.757 | 46.218 | 41.692 | 1.00 72.74 | AAAA |
| ATOM | 95 | CE | LYS | 14 | 42.183 | 45.639 | 40.336 | 1.00 67.25 | AAAA |
| | 96 | NZ | LYS | 14 | 41.637 | 44.280 | 40.045 | 1.00 70.06 | AAAA |
| MOTA | | | LYS | 14 | 39.589 | 42.688 | 42.834 | 1.00 39.98 | AAAA |
| MOTA | 97 | C | | | 39.746 | 42.350 | 41.658 | 1.00 46.99 | AAAA |
| MOTA | 98 | 0 | LYS | 14 | | | | 1.00 32.64 | AAAA |
| ATOM | 99 | N | TYR | 15 | 38.927 | 41.944 | 43.717 | | |
| ATOM | 100 | CA | TYR | 15 | 38.318 | 40.655 | 43.355 | 1.00 41.01 | AAAA |
| MOTA | 101 | CB | TYR | 15 | 38.996 | 39.512 | 44.126 | 1.00 26.48 | AAAA |
| ATOM | 102 | CG | TYR | 15 | 40.496 | 39.571 | 44.033 | 1.00 34.97 | AAAA |
| ATOM | 103 | | TYR | 15 | 41.289 | 39.401 | 45.167 | 1.00 43.28 | AAAA |
| | 104 | CE1 | TYR | 15 | 42.677 | 39.548 | 45.106 | 1.00 36.05 | AAAA |
| MOTA | 105 | CD2 | TYR | 15 | 41.127 | 39.879 | 42.827 | 1.00 40.78 | AAAA |
| ATOM | | | | 15 | 42.508 | 40.027 | 42.756 | 1.00 37.13 | AAAA |
| MOTA | 106 | CE2 | TYR | | | 39.865 | 43.899 | 1.00 36.87 | AAAA |
| MOTA | 107 | CZ | TYR | 15 | 43.275 | | | | AAAA |
| ATOM | 108 | OH | TYR | 15 | 44.644 | 40.044 | 43.844 | 1.00 35.40 | |
| MOTA | 109 | С | TYR | 15 | 36.838 | 40.705 | 43.714 | 1.00 38.62 | AAAA |
| ATOM | 110 | 0 | TYR | 15 | 36.344 | 39.868 | 44.468 | 1.00 37.82 | AAAA |
| ATOM | 111 | N | ARG | 16 | 36.141 | 41.703 | 43.177 | 1.00 44.85 | AAAA |
| | 112 | CA | ARG | 16 | 34.716 | 41.890 | 43.431 | 1.00 45.75 | AAAA |
| ATOM | | | ARG | 16 | 34.320 | 43.348 | 43.187 | 1.00 54.17 | AAAA |
| ATOM | 113 | CB CG | ARG | 16 | 35.170 | 44.399 | 43.875 | 1.00 66.77 | AAAA |
| ATOM | 114 | | | | | 44.506 | 45.369 | 1.00 72.39 | AAAA |
| MOTA | 115 | CD | ARG | 16 | 34.920 | | 45.923 | 1.00 72.39 | AAAA |
| ATOM | 116 | NE | ARG | 16 | 35.649 | 45.646 | | | |
| ATOM | 117 | CZ | ARG | 16 | 35.489 | 46.906 | 45.518 | 1.00 81.94 | AAAA |
| ATOM | 118 | NH1 | ARG | 15 | 34.624 | 47.197 | 44.554 | 1.00 80.19 | AAAA |
| MOTA | 119 | | ARG | 16 | 36.205 | 47.878 | 46.069 | 1.00 85.46 | AAAA |
| | 120 | C | ARG | 16 | 33.915 | 41.029 | 42.460 | 1.00 43.50 | AAAA |
| ATOM | | | | | 34.400 | 40.667 | 41.385 | 1.00 38.62 | AAAA |
| MOTA | 121 | 0 | ARG | 16 | | | 42.833 | 1.00 32.68 | AAAA |
| MOTA | 122 | N | TYR | 17 | 32.689 | 40.692 | | 1.00 32.68 | AAAA |
| ATOM | 123 | CA | TYR | 17 | 31.850 | 39.923 | 41.930 | | |
| ATOM | 124 | CB | TYR | 17 | 30.662 | 39.306 | 42.672 | 1.00 41.05 | AAAA |
| ATOM | 125 | CG | TYR | 17 | 31.040 | 38.104 | 43.519 | 1.00 37.51 | AAAA |
| | 126 | | TYR | 17 | 32.039 | 38.194 | 44.493 | 1.00 32.59 | AAAA |
| ATOM | 127 | | TYR | 17 | 32.383 | 37.095 | 45.277 | 1.00 29.32 | AAAA |
| ATOM | | | | 17 | 30.393 | 36.875 | 43.346 | 1.00 31.46 | AAAA |
| ATOM | 128 | | TYR | | | | 44.122 | 1.00 28.64 | AAAA |
| ATOM | 129 | | TYR | 17 | 30.726 | 35.772 | | 1.00 28.04 | AAAA |
| ATOM | 130 | CZ | TYR | 17 | 31.721 | 35.887 | 45.088 | 1.00 27.14 | AAAA |
| ATOM | 131 | ОН | TYR | 17 | 32.044 | 34.807 | 45.881 | 1.00 21.73 | |
| ATOM | 132 | C | TYR | 17 | 31.380 | 40.871 | 40.836 | 1.00 40.97 | AAAA |
| | | | | | | | - | | • |

| | 122 | 0 | TYR | 17 | 31.435 | 42.097 | 40.984 | 1.00 29.58 | AAAA |
|--------|-----|-----|-------|------|--------|--------|---------|------------|----------------|
| ATCM | 133 | | | | 30.904 | 40.321 | 39.722 | 1.00 41.02 | AAAA |
| ATCM | 134 | N | PPO | 18 | - | | | 1.00 48.67 | AAAA |
| ATOM | 135 | CD | PRO | 18 | 30.760 | 38.910 | 39.318 | | |
| | | | PRO | 18 | 30.459 | 41.197 | 38.649 | 1.00 49.35 | AAAA |
| MOTA | 136 | CA | | | 30.321 | 40.228 | 37.481 | 1.00 59.04 | AAAA |
| ATOM | 137 | CB | PRO | 18 | | | | | AAAA |
| ATOM | 138 | CG | PRO | 18 | 29.756 | 39:017 | 38.179 | 1.00 54.15 | |
| | | | | 18 | 29.178 | 41.982 | 38.864 | 1.00 54.97 | AAAA |
| ATOM | 139 | С | PRO | | | | 39.850 | 1.00 46.85 | AAAA |
| ATOM | 140 | 0 | PRO | 18 | 28.457 | 41.823 | | | |
| | | N | LYS | 19 | 28.961 | 42.868 | 37.904 | 1.00 60.87 | AAAA |
| MOTA | 141 | | | | 27.777 | 43.696 | 37.749 | 1.00 67.78 | AAAA |
| MOTA | 142 | CA | LYS | 19 | | | | 1.00 73.26 | AAAA |
| ATOM | 143 | CB | LYS | 19 - | 27.155 | 43.278 | 36.425 | | |
| | | | LYS | 19 | 26.971 | 41.752 | 36.414 | 1.00 77.87 | AAAA |
| MOTA | 144 | CG | | | | 41.166 | 35.209 | 1.00 81.01 | AAAA |
| ATOM | 145 | CD | LYS | 19 | 26.276 | | | 1.00 82.45 | AAAA |
| ATOM | 146 | CE | LYS | 19 | 26.039 | 39.680 | 35.471 | | |
| - | | | LYS | 19 | 25.417 | 38.959 | 34.331 | 1.00 83.11 | AAAA |
| ATOM | 147 | NZ | | | | 43.594 | 38.814- | 1.00 64.15 | AAAA |
| MOTA | 148 | С | LYS | 19 | 26.688 | | | 1.00 65.73 | AAAA |
| | 149 | 0 | LYS | 19 | 26.810 | 44.047 | 39.949 | | |
| MOTA | | | ASN | 20 | 25.604 | 42.986 | 38.345 | 1.00 59.78 | AAAA |
| ATOM | 150 | N | | | | 42.703 | 39.025 | 1.00 59.91 | AAAA |
| ATOM | 151 | CA | ASN | 20 | 24.353 | | | | AAAA |
| | 152 | CB | ASN | 20 | 23.516 | 41.844 | 38.077 | 1.00 68.08 | |
| ATOM | | | ASN | 20 | 22.108 | 42.355 | 37.907 | 1.00 78.73 | AAAA |
| ATOM | 153 | CG | | | | 43.498 | 37.496 | 1.00 78.67 | AAAA |
| MOTA | 154 | OD1 | ASN | 20 | 21.894 | | | 1.00 70.07 | AAAA |
| | 155 | MD2 | ASN | 20 | 21.132 | 41.505 | 38.211 | 1.00 83.22 | |
| ATOM | | | | 20 | 24.474 | 41.977 | 40.361 | 1.00 53.35 | AAAA |
| ATOM | 156 | С | ASN | | | | 41.234 | 1.00 59.92 | AAAA |
| MOTA | 157 | 0 | ASN | 20 | 23.611 | 42.112 | | | |
| | 158 | N | HIS | 21 | 25.543 | 41.206 | 40.511 | 1.00 44.23 | AAAA |
| ATOM | | | | | 25.768 | 40.397 | 41.707 | 1.00 28.15 | AAAA |
| ATOM | 159 | CA | HIS | 21 | | | 41.570 | 1.00 31.84 | AAAA |
| ATOM | 160 | CB | HIS | 21 | 27.088 | 39.639 | | | |
| | 161 | CG | HIS | 21 | 27.155 | 38.411 | 42.418 | 1.00 34.79 | AAAA |
| MCTA | | | | 21 | 27.344 | 38.259 | 43.752 | 1.00 25.03 | AAAA |
| ATOM ' | 162 | | HIS | | | | 41.917 | 1.00 34.81 | AAAA |
| ATOM | 163 | ND1 | HIS | 21 | 26.929 | 37.148 | | | AAAA |
| | 164 | | HIS | 21 | 26.979 | 36.269 | 42.900 | 1.00 17.01 | |
| MOTA | | | | 21 | 27.228 | 36.917 | 44.026 | 1.00 32.31 | AAAA |
| MOTA | 165 | NE2 | HIS | | _ | | 43.051 | 1.00 29.37 | AAAA |
| ATOM | 166 | С | HIS | 21 | 25.763 | 41.135 | | | AAAA |
| | 167 | 0 | HIS | .21 | 26.346 | 42.210 | 43.186 | 1.00 28.54 | |
| ATOM | | | PRO | 22 | 25.093 | 40.565 | 44.066 | 1.00 29.14 | AAAA |
| ATOM | 168 | N | | | | 39.322 | 44.061 | 1.00 31.20 | AAAA |
| ATOM | 169 | CD | PRO | 22 | 24.301 | | | 1.00 32.84 | AAAA |
| ATOM | 170 | CA | PRO | 22 | 25.034 | 41.185 | 45.395 | | |
| | | | | 22 | 24.174 | 40.192 | 46.187 | 1.00 34.98 | AAAA |
| ATOM | 171 | CB | PRO | | 23.257 | 39.634 | 45.109 | 1.00 30.11 | AAAA |
| ATOM | 172 | CG | PRO | 22 | | | | 1.00 34.37 | AAAA |
| ATOM | 173 | С | PRO | 22 | 26.411 | 41.415 | 46.044 | 1.00 34.37 | |
| | | | PRO | 22 | 26.554 | 42.272 | 46.916 | 1.00 29.17 | AAAA |
| ATOM | 174 | 0 | | | 27.415 | 40.644 | 45.629 | 1.00 29.22 | AAAA |
| ATOM | 175 | N | LEU | 23 | _ | | | 1.00 26.49 | AAAA |
| ATOM | 176 | CA | LEU | 23 | 28.765 | 40.781 | 46.181 | | |
| | | CB | LEU | 23 | 29.414 | 39.397 | 46.332 | 1.00 22.30 | AAAA |
| atom | 177 | | | | 28.703 | 38.527 | 47.380 | 1.00 21.04 | AAAA |
| ATOM | 178 | CG | LEU | 23 | | | 47.410 | 1.00 19.35 | AAAA |
| ATOM | 179 | CD1 | LEU | 23 | 29.307 | 37.113 | | 1.00 19.55 | AAAA |
| | | CD3 | LEU | 23 | 28.850 | 39.197 | 48.746 | 1.00 26.51 | |
| ATOM | 180 | | | | 29.561 | 41.718 | 45.361 | 1.00 25.81 | AAAA |
| ATOM | 181 | С | LEU | 23 | | | | 1.00 28.45 | AAAA |
| ATOM | 182 | С | LEU | 23 | 30.893 | 41.693 | 45.477 | | |
| | | N | LYS | 24 | 29.018 | 42.539 | 44.532 | 1.00 24.86 | AAAA |
| ATOM | 183 | | | | 29.696 | 43.552 | | 1.00 27.35 | AAAA |
| ATOM | 184 | ÇA | LYS | 24 | 29.030 | | | 1.00 28.57 | AAAA |
| ATOM | 185 | CB | LYS | 24 | 28.662 | 44.244 | | 1.00 28.37 | AAAA |
| | | | LYS | 24 | 29.118 | 45.532 | 42.171 | 1.00 52.95 | |
| atom | 186 | CG | | | 28.025 | 46.603 | | 1.00 63.74 | AAAA |
| ATOM | 187 | CD | LYS | 24 | | | | 1.00 66.09 | AAAA |
| ATOM | 188 | CE | LYS | 24 | 26.688 | 46.138 | | | |
| | | | LYS | 24 | 25.595 | 47.137 | 41.896 | 1.00 66.00 | AAAA |
| ATOM | 189 | ΝZ | | | 30.332 | 44.592 | | | AAAA |
| ATOM | 190 | Ç | LYS | 4 4 | | | | | AAAA |
| ATOM | 191 | 0 | LYS | 24 | 31.412 | 45.123 | | | |
| | | | ILE | 25 | 29.652 | 44.879 | 45.779 | 1.00 26.90 | AAAA |
| ATOM | 192 | N | | | 30.151 | 45.865 | | | AAAA |
| ATOM | 193 | CA | ILE | 25 | | | | | AAAA |
| ATOM | 194 | СВ | ILE | 25 | 29.105 | 46.177 | | 4 | |
| | | | | 25 | 27.961 | 46.951 | 47.237 | 1.00 23.84 | AAAA |
| ATOM | 195 | | 2 ILE | | - | 44.869 | | | AAAA |
| ATOM | 196 | CG: | I ILE | 25 | 28.661 | | | | ` AAA A |
| ATOM | 197 | CD1 | ILE | 25 | 27.718 | 45.051 | | | |
| | | | ILE | | 31.424 | 45.463 | 47.483 | 1.00 32.19 | AAAA |
| -TCM | 198 | _ | ت ب | | | | • | | • |
| , | | | • | | | | | | |

| ATOM | 199 | 0 | ILE | 25 | 31.736 | 44.271 | 47.623 | 1.00 26.54 | AAAA |
|--------|------------|----------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 200 | N | PRO | 26 | 32.191 | 46.463 | 47.956 | 1.00 30.14 | AAAA |
| ATOM | 201 | CD | PRO | 26 | 31.979 | 47.907 | 47.770 | 1.00 36.38 | AAAA |
| ATOM | 202 | CA | PRO | 26 | 33.431 | 46.241 | 48.707 | 1.00 30.63 | AAAA |
| ATOM | 203 | CB | PRO | 26 | 34.014 | 47.652 | 48.814 | 1.00 34.29 | AAAA |
| ATOM - | 204 | CG | PRO | 26 | 33.397 | 48.373 | 47.617 | 1.00 43.39 | AAAA |
| ATOM | 205 | c | PRO | 26 | 32.943 | 45.727 | 50.061 | 1.00 25.99 | AAAA |
| ATOM | 206 | Ö | PRO | 26 | 31.854 | 46.110 | 50.484 | 1.00 25.51 | ÁAAA |
| ATOM | 207 | N | ARG | 27 | 33.719 | 44.880 | 50.743 | 1.00 21.98 | AAAA |
| ATOM | 208 | CA | ARG | 2.7 2.7 | 33.267 | 44.347 | 52.035 | 1.00 26.17 | AAAA |
| ATOM | 209 | CB | ARG | 27 | 32.641 | 42.969 | 51.834 | 1.00 22.70 | AAAA |
| ATOM | 210 | CG | ARG | 27 | 31.442 | 43.039 | 50.890 | 1.00 26.75 | AAAA |
| ATOM | 211 | CD | ARG | 27 · | 30.832 | 41.672 | 50.581- | | AAAA |
| ATOM | 212 | NE | ARG | 27 | 30.121 | 41.098 | 51.716 | 1.00 28.66 | AAAA |
| ATOM | 213 | CZ | ARG | 27 | 30.582 | 40.129 | 52.503 | 1.00 31.79 | AAAA |
| ATOM | 214 | | ARG | 27 | 31.778 | 39.598 | 52.290 | 1.00 34.08 | AAAA - |
| ATOM | 215 | | ARG | 27 | 29.833 | 39.688 | 53.505 | 1.00 26.16 | AAAA |
| ATOM | 216 | С | ARG | 27 | 34.358 | 44:297 | 53.090 | 1.00 24.10 | AAAA |
| ATOM | 217 | ŏ | ARG | 27 | 34.326 | 45.074 | 54.038 | 1.00 23.50 | AAAA |
| MOTA | 218 | N | VAL | 28 | 35.314 | 43.390 | 52.960 | 1.00 21.45 | AAAA |
| ATOM | 219 | CA | VAL | 28 | 36.385 | 43.385 | 53.953 | 1.00 21.75 | AAAA |
| ATOM | 220 | CB | VAL | 28 | 37.221 | 42.101 | 53.866 | 1.00 26.55 | AAAA |
| MOTA | 221 | | VAL | 28 | 38.407 | 42.177 | 54.830 | 1.00 23.84 | AAAA |
| ATOM | 222 | | VAL | 28 | 36.337 | 40.906 | 54.214 | 1.00 19.20 | AAAA |
| ATOM | 223 | c | VAL | 28 | 37.277 | 44.611 | 53.736 | 1.00 20.86 | AAAA |
| ATOM | 224 | Ō | VAL | 28 | 37.770 | 45.223 | 54.702 | 1.00 25.15 | AAAA |
| ATOM | 225 | N | SER | 29 | 37.480 | 44.996 | 52.475 | 1.00 19.22 | AAAA |
| ATOM | 226 | CA | SER | 29 . | 38.320 | 46.169 | 52.209 | 1.00 19.63 | AAAA |
| ATOM | 227 | CB | SER | 29 | 38.591 | 46.352 | 50.702 | 1.00 24.45 | AAAA |
| ATOM | 228 | OG | SER | 29 | 37.411 | 46.697 | 49.984 | 1.00 28.74 | AAAA |
| ATOM | 229 | С | SER | 29 | 37.579 | 47.381 | 52.756 | 1.00 21.50 | AAAA |
| ATOM | 230 | 0 | SER | 29 | 38.184 | 48.320 | 53.271 | 1.00 18.95 | AAAA |
| ATOM | 231 | N | LEU | 30 | 36.256 | 47.353 | 52.673 | 1.00 19.56 | AAAA |
| MOTA | 232 | CA | LEU | 30 | 35.499 | 48.481 | 53.177 | 1.00 25.97 | AAAA |
| ATOM | 233 | CB | LEU | 30 | 34.032 | 48.396 | 52.744 | 1.00 22.90 | AAAA |
| MOTA | 234 | CG | LEU | 30 | 33.085 | 49.541 | 53.157 | 1.00 26.62 | AAAA |
| MOTA | 235 | | LEU | 30 | 32.885 | 49.539 | 54.648 | 1.00 38.27 | AAAA |
| MOTA | 236 | CD2 | LEU | 30 | 33.653 | 50.885 | 52.698 | 1.00 25.71 | AAAA |
| ATOM | 237 | С | LEU | 30 | 35.604 | 48.509 | 54.696 | 1.00 18.44 | AAAA |
| ATOM . | 238 | 0 | LEU | 30 | 35.704 | 49.580 | 55.273 | 1.00 25.05 | AAAA |
| MOTA | 239 | N | LEU | 31 | 35.578 | 47.336 | 55.336 | 1.00 19.65 | AAAA AAAA |
| MOTA | 240 | CA | LEU | 31 | 35.672 | 47.270 | 56.797 | 1.00 20.47 1.00 20.60 | AAAA |
| ATOM | 241 | CB | LEU | 31 | 35.613 | 45.821 | 57.300 | 1.00 20.80 | AAAA |
| MOTA | 242 | CG | LEU | 31 | 34.988 | 45.456 | 58.665 | 1.00 33.80 | AAAA |
| MOTA | 243 | | LEU | 31 | 35.712 | 44.219 | 59.257 59.637 | 1.00 23.33 | AAAA |
| MOTA | 244 | | LEU | 31 | 35.085 | 46.591 | 57.229 | 1.00 23.85 | AAAA |
| MOTA | 245 | C | LEU | 31 | 37.009 | 47.870 48.673 | 58.154 | 1.00 21.24 | AAAA |
| ATOM | 346 | 0 | LEU | 31 | 37.070 | 47.462 | 56.562 | 1.00 23.91 | AAAA |
| ATOM | 247 | N | LEU | 32 | 38.079 39.400 | 47.965 | 56.899 | 1.00 24.82 | AAAA |
| ATOM | 248 | CA | LEU | 32 | 40.479 | 47.320 | 56.018 | 1.00 24.81 | AAAA |
| MOTA | 249 | CB | LEU | 32 | 40.849 | 45.854 | 56.276 | 1.00 27.00 | AAAA |
| ATOM | 250 | CG | LEU | 32 32 | 41.995 | 45.435 | 55.354 | 1.00 27.13 | AAAA |
| MOTA | 251 | | | 32 | 41.285 | 45.687 | 57.720 | 1.00 34.49 | AAAA |
| | . 252 | | LEU | 32 | 39.466 | 49.475 | 56.763 | 1.00 19.56 | AAAA |
| ATOM | 253 | C | LEU LEU | 32 | 39.958 | 50.143 | 57.662 | 1.00 20.71 | AAAA |
| ATOM | 254 | 0 | | 33 | 38.974 | 50.006 | 55.645 | 1.00 23.25 | AAAA |
| ATOM | 255 | N | ARG | 33 | 39.007 | 51.449 | 55.441 | 1.00 24.33 | AAAA |
| ATOM | | · CA | ARG | 33 | 38.575 | 51.806 | 54.013 | 1.00 23.46 | AAAA |
| ATOM | 257 | CB | ARG | 33 | 39.571 | 51.327 | 52.945 | 1.00 26.94 | AAAA |
| ATOM | 258 | CG | ARG | 33 | 39.337 | 51.976 | 51.585 | 1.00 42.13 | AAAA |
| ATOM | 259 260 | CD NE | ARG ARG | 33 | 38.023 | 51.661 | 51.037 | 1.00 59.06 | AAAA |
| ATOM | | CZ | ARG | 33 | 37.583 | 52.088 | 49.857 | 1.00 60.87 | AAAA |
| ATOM | 261 262 | | ARG | 33 | 38.353 | 52.850 | 49.095 | 1.00 65.33 | AAAA |
| ATOM | 263 | | ARG | 33 | 36.373 | 51.743 | 49.433 | 1.00 56.24 | AAAA |
| ATOM | 264 | C | ARG | 33 | 38.124 | 52.156 | 56.455 | 1.00 30.33 | AAAA |
| MOTA | 04 | ٠. | D/A | J J | | | • | | • |

| | | | _ | • | 38.441 | 5 | 3.252 | 56.905 | 1.00 2 | 5.45 | AAAA |
|------|--------------|-------|------------|----|-----------------|-----|----------------|--------|--------|---------|-------|
| ATOM | 265 0 | AI | | 33 | 37.022 | 5 5 | | 56.828 | 1.00 2 | 4.98 | AAAA |
| MOTA | 266 N | | ΞE | 34 | 36.099 | | | 57.789 | 1.00 2 | 7.09 | AAAA |
| MOTA | 267 C. | | HE | 34 | 34.798 | | 1.276 | 57.807 | 1.00 2 | 4.88 | AAAA |
| MOTA | 268 C | | HE | 34 | 33.719 | | 1.898 | 58.631 | 1.00 2 | 0.46 | AAAA |
| ATOM | 269 C | | HE. | 34 | 33.043 | | 3.018 | 58.171 | 1.00 1 | 18.74 | AAAA |
| MOTA | | D1 PI | | 34 | 33.39 | | 1.383 | 59.889 | 1.00 2 | 20.19 | AAAA |
| ATOM | - · - | D2 PI | | 34 | | | 3.627 | 58.956 | 1.00 2 | 23.04 | AAAA |
| MOTA | | El P | | 34 | 32.043 32.40 | | 1.974 | 60.681 | 1.00 2 | 25.08 | AAAA |
| ATOM | | | HE · | 34 | 31.72 | | 3.104 | 60.209 | 1.00 | 23.31 | AAAA |
| ATOM | 274 C | | HE | 34 | 36.70 | - | 2.115 | 59.194 | 1.00 2 | 23.93 | AAAA |
| ATOM | 275 C | | HE | 34 | 36.66 | | 3.138 | 59.883 | 1.00 | 21.71 | AAAA |
| MOTA | 276 0 | | HE | 34 | 37.29 | | 1.013 | 59.645 | 1.00 | 21.33 | AAAA |
| ATOM | 277 N | | YS | 35 | 37.86 | | 1.084 | 60.978 | 1.00 | 22.54 | AAAA |
| MOTA | | | YS | 35 | 38.27 | | 19.716 | 61.476 | 1.00 | 29.70 | AAAA |
| ATOM | 279 C | | YS | 35 | 37.08 | _ | 18.890 | 61.924 | 1.00 | 29.48 | AAAA |
| ATOM | | - | YS | 35 | | _ | 17.535 | 62.398 | 1.00 | 42.17 | AAAA |
| MOTA | 281 | | YS | 35 | 37.51 | | 46.762 | 61.275 | 1.00 | 34.89 | AAAA |
| ATOM | 282 C | | YS | 35 | 38.15 | | 47.412 | 60.719 | 1.00 | 67.18 | AAAA |
| ATOM | 283 N | | YS. | 35 | 39.37 | | 52.055 | 61.040 | 1.00 | 24.68 | AAAA |
| MOTA | 284 | - | YS. | 35 | 39.02 | | 52.640 | 62.085 | 1.00 | 22.33 | AAAA |
| ATOM | 285 | | .YS | 35 | 39.28 | _ | 52.231 | 59.926 | 1.00 | 25.67 | AAAA |
| ATOM | 286 1 | ائر 1 | SP | 36 | 39.72 | | 53.163 | 59.898 | 1.00 | 25.57 | AAAA |
| ATOM | 287 | | SP | 36 | 40.84 | | 52.984 | 58.621 | 1.00 | 32.26 | AAAA |
| MOTA | 288 (| | SP | 36 | 41,66 | | 53.914 | 58.572 | 1.00 | 33.92 | AAAA |
| ATOM | | | SP | 36 | 42.88 43.64 | _ | 53.969 | 59.563 | 1.00 | 40.22 | AAAA |
| ATOM | | DD1 A | | 36 | | _ | 54.575 | 57.538 | 1.00 | 40.06 | AAAA |
| ATOM | 291 | DD2 A | | 36 | 43.07 | _ | 54.578 | 59.973 | 1.00 | 28.04 | AAAA |
| ATOM | 292 | | ASP | 36 | 40.28 | | 55.397 | 60.765 | 1.00 | 29.52 | AAAA |
| MOTA | 293 | | ASP | 36 | 40.76 39.27 | - | 54.864 | 59.159 | 1.00 | 23.32 | AAAA |
| ATOM | 294 | | ALA | 37 | | | 56.192 | 59.163 | 1.00 | 28.22 | AAAA |
| MOTA | 295 | | ALA | 37 | 38.65 | | 56.251 | 58.119 | 1.00 | 25.93 | AAAA |
| ATOM | 296 | | ALA | 37 | 37.50 | | 56.549 | 60.565 | 1.00 | 28.41 | AAAA |
| ATOM | 297 | - | ALA | 37 | 38.12 | | 57.708 | 60.972 | 1.00 | 29.27 | AAAA |
| ATOM | 298 | | ALA | 37 | 38.18 | | 55.547 | 61.300 | 1.00 | 24.76 | AAAA |
| ATOM | 299 | | MET | 38 | 37.63 37.10 | | 55.727 | 62.669 | 1.00 | 25.45 | AAAA |
| ATOM | 300 | | MET | 38 | | | 54.625 | 62.982 | 1.00 | 25.19 | AAAA |
| ATOM | | | MET | 38 | 36.0 | | 54.660 | 62.148 | | 22.32 | AAAA |
| MOTA | 302 | | MET | 38 | 34.83 33.73 | | 55.983 | 62.702 | 1.00 | 29.90 | AAAA |
| ATOM | 303 | | MET | 38 | 33.4 | | 55.417 | 64.376 | 1.00 | 26.51 | AAAA |
| ATOM | | | MET | 38 | 38.2 | | 55.667 | 63.744 | 1.00 | 26.42 | AAAA |
| MOTA | 305 | - | MET | 38 | 37.9 | | 55.818 | 64.947 | 1.00 | 23.77 | AAAA |
| MOTA | 306 | | MET | 38 | 39.4 | | 55.434 | 63.300 | 1.00 | 26.21 | AAAA |
| MOTA | 307 | | ASN | 39 | 40.6 | | 55.308 | 64.170 | 1.00 | 28.53 | AAAA |
| MOTA | 308 | | ASN | 39 | 40.9 | | 56.643 | 64.855 | 1.00 | 33.95 | AAAA |
| ATOM | 309 | | ASN | 39 | 41.1 | | 57.751 | 63.858 | 1.00 | 29.46 | AAAA |
| ATOM | 310 | ~~ | ASN | 39 | 41.1 | | 57.596 | 62.925 | 1.00 | 36.28 | AAAA |
| MOTA | 311 | OD1 | | 39 | 40.4 | | 58.880 | | 1.00 | 40.03 | AAAA |
| MOTA | 312 | ND2 | | 39 | 40.3 | | 54.223 | | 1.00 | 30.07 | AAAA |
| ATOM | 313 | | ASN | 39 | 40.6 | | 54.390 | | 1.00 | 25.47 | AAAA |
| MOTA | 314 | | ASN | 39 | 39.8 | | 53.105 | | 1.00 | 28.19 | AAAA |
| ATOM | 315 | | LEU | 40 | 39.5 | | 51.984 | | 1.00 | 25.50 | AAAA |
| ATOM | 316 | CA | LEU | 40 | 38.0 | | 51.562 | | 1.00 | 32.14 | AAAA |
| ATOM | 317 | CB | LEU | 40 | 37.0 | | 52,585 | | 1.00 | 30.47 | AAAA |
| ATOM | 318 | CG | LEU | 40 | 37.6 35.6 | | 52.027 | | 1.00 | 29.07 | AAAA. |
| ATOM | 319 | CD1 | LEU | 40 | 37.3 | | 52.889 | | 1.00 | 23.80 | AAAA |
| MOTA | 320 | CD2 | | 40 | | | 50.771 | | 1.00 | 26.99 | AAAA |
| ATOM | 321 | C | LEU | 40 | 40.4 | | 49.683 | | 1.00 | 25.41 | AAAA |
| ATOM | 322 | 0 | LEU | 40 | 40.1 | | 50.970 | | 1.00 | 0 28.33 | AAAA |
| ATOM | 323 | N | ILE | 41 | 41.5 | | 49.882 | · | 1.00 | 0 25.08 | AANA |
| ATOM | 324 | CA | ILE | 41 | 42.4 | | 49.02 | | 3 1.0 | 0 25.01 | AAAA |
| ATCM | 325 | CB | ILE | 41 | 42.0 | | 49.02 | | 1.0 | 0 22.74 | AAAA |
| ATOM | 326 | CG2 | ILE | 41 | 42.0 | | 47.80 | | 3 1.0 | 0 31.01 | AAAA |
| ATOM | 327 | CG1 | ILE | 41 | 42.5 | | 46.95 | | | 0 42.18 | AAAA |
| ATCM | 328 | | ILE | 41 | 42. | | | | 7 1.0 | 0 24.09 | AAAA |
| ATOM | 329 | С | ILE | 41 | 43. | | 50.37 51.40 | | | 0 28.92 | AAAA |
| ATOM | 330 | 0 | ILE | 41 | 44. | 140 | J1.40 | | | | • |
| | | | | | | | | | | | |

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|--------|-----------|--------|-------------|--------|------------|------------|--------|
| | 331 N A | SP 42 | 44.866 | 49.634 | | 1.00 28.95 | AAAA |
| ATOM | | SP 42 | 46.279 | 49.988 | | 1.00 32.52 | AAAA |
| ATOM | | SP 42 | 46.951 | 50.094 | | 1.00 34.24 | AAAA |
| ATOM | • • - | SP 42 | 46.267 | 51.097 | 66.911 | 1.00 51.23 | AAAA |
| MOTA | | | 46.079 | 52.250 | 66.467 | 1.00 50.19 | AAAA |
| ATOM | 335 OD1 A | | 45.924 | 50.736 | 68.062 | 1.00 53.00 | AAAA |
| ATOM | 336 OD2 A | | 46.985 | 48.919 | 63.808 | 1.00 31.13 | AAAA |
| MOTA | | SP 42 | | 47.758 | 63.838 | 1.00 26.71 | AAAA |
| ATOM | | SP 42 | 46.594 | | 63.092 | 1.00 29.99 | AAAA |
| ATOM | 339 N G | LU 43 | 48.036 | 49.312 | 62.240 | 1.00 31.34 | AAAA |
| ATOM | | LU 43 | 48.793 | 48.392 | | 1.00 36.12 | AAAA |
| ATOM | 341 CB G | LU 43 | 50.078 | 49.045 | 61.724 | 1.00 52.72 | AAAA |
| ATOM | | LU 43 | 49.886 | 50.118 | 60.676 | | AAAA |
| | | LU 43 | 51.214 | 50.556 | 60.083 | 1.00 60.39 | AAAA |
| ATOM | 344 OE1 G | | 51.928 | 49.688 | 59.536 | 1.00 70.32 | AAAA |
| MOTA | 345 OE2 G | - | 51.550 | 51.755 | 60.163 | 1.00 60.38 | |
| MOTA | | LU 43 | 49.196 | 47.070 | 62.859 | 1.00 38.04 | AAAA |
| ATOM . | | LU 43 | 49.125 | 46.024 | 62.209 | 1.00 36.83 | AAAA |
| ATOM | • • • | | 49.636 | 47.103 | 64.105 | 1.00 28.26 | AAAA |
| ATOM | | | 50.084 | 45.879 | 64.740 | 1.00 32.71 | AAAA |
| MOTA | | YS 44 | 50.974 | 46.245 | 65.927 | 1.00 44.28 | AAAA |
| ATOM | • | xs 44 | 52.211 | 47.007 | 65.418 | 1.00 59.37 | AAAA |
| MOTA | | YS 44 | | 47.449 | 66.491 | 1.00 68.87 | AAAA |
| ATOM | | YS 44 | 53.187 | 48.167 | 65.849 | 1.00 67.21 | AAA£. |
| MOTA | 353 CE L | YS 44 | 54.373 | | 66.850 | 1.00 74.00 | AAAA |
| ATOM | 354 NZ I | LYS 44 | 55.361 | 48.648 | | 1.00 26.75 | AAAA |
| ATOM | | LYS 44 | 48.982 | 44.889 | 65.115 | 1.00 27.37 | AAAA |
| MOTA | | LYS 44 | 49.265 | 43.792 | 65.586 | 1.00 27.37 | AAAA |
| ATOM | | GLU 45 | 47.731 | 45.278 | 64.881 | 1.00 23.20 | AAAA |
| | | GLU 45 | 46.580 | 44.414 | 65.165 | 1.00 21.58 | AAAA |
| MOTA | | GLU 45 | 45.387 | 45.243 | 65.676 | 1.00 18.24 | |
| MOTA | | GLU 45 | 45.551 | 45.828 | 67.077 | 1.00 26.57 | AAAA |
| MOTA | | GLU 45 | 44.418 | 46.772 | 67.453 | 1.00 23.12 | AAAA |
| MOTA | | | 44.224 | 47.783 | 66.746 | 1.00 21.64 | AAAA |
| ATOM | • | | 43.725 | 46.509 | 68.454 | 1.00 26.48 | AAAA |
| ATOM | 363 OE2 0 | | | 43.710 | 63.870 | 1.00 26.31 | AAAA |
| MOTA | • • • • | | 45.400 | 42.739 | 63.889 | 1.00 22.32 | AAAA |
| MOTA | • | GLU 45 | | 44.204 | 62.748 | 1.00 20.15 | AAAA |
| ATOM | | LEU 46 | 46.317 | 43.642 | 61.448 | 1.00 25.80 | AAAA |
| ATOM | | LEU 46 | | 44.774 | 60.433 | 1.00 27.25 | AAAA |
| ATOM | | LEU 46 | 46.137 | 44.397 | 58.997 | 1.00 37.72 | AAAA |
| MOTA | | LEU 46 | 45.763 | | 58.984 | 1.00 39.46 | AAAA |
| ATOM | 370 CD1 | | 44.356 | 43.810 | 58.101 | 1.00 35.43 | AAAA |
| ATOM | 371 CD2 | LEU 46 | 45.822 | 45.632 | 60.896 | 1.00 28.88 | AAAA |
| MOTA | 372 C | LEU 46 | 47.305 | 42.623 | | 1.00 31.98 | AAAA |
| MOTA | | LEU 46 | 48.513 | 42.860 | 60.862 | 1.00 16.92 | AAAA |
| ATOM | | ILE 47 | 46.791 | 41.469 | 60.482 | 1.00 20.98 | AAAA |
| MOTA | | ILE 47 | 47.638 | 40.448 | 59.872 | 1.00 20.50 | AAAA |
| ATOM | | ILE 47 | 47.412 | 39.046 | | 1.00 21.31 | AAAA |
| | 377 CG2 | | 48.115 | 37.958 | 53.696 | 1.00 20.32 | AAAA |
| ATOM | 378 CG1 | | 47.947 | 39.040 | € .950 | 1.00 20.71 | AAAA |
| MOTA | 379 CD1 | | 49.450 | 39.207 | | 1.00 38.87 | |
| ATOM | | ILE 47 | 47.227 | 40.417 | | 1.00 24.50 | AAAA |
| ATOM | • • - | | | | 58.101 | 1.00 20.74 | AAAA |
| ATOM | _ | | | 40.550 | 57.500 | 1.00 18.73 | AAAA |
| atom | | | | 40.543 | 56.072 | 1.00 15.55 | AAAA |
| ATOM | | LYS 48 | | | | 1.00 16.52 | AAAA |
| MOTA | | LYS 48 | | | | 1.00 23.25 | AAAA |
| MOTA | | LYS 48 | | | | 1.00 32.69 | AAAA |
| MOTA | | LYS 48 | | | | | AAAA |
| ATOM | 387 CE | LYS 48 | | | | | AAAA |
| ATOM | 388 NZ | LYS 48 | | | | | AAAA |
| ATOM | 389 C | LYS 48 | 47.473 | 39.140 | | | AAAA |
| | 390 0 | LYS 48 | 48.177 | | 55.887 | 1.00 16.63 | AAAA |
| MOTA | 391 N | SER 49 | | | | | AAAA |
| ATCM | 392 CA | SER 49 | 45.838 | 37.780 | | | AAAA · |
| ATOM | | SER 45 | | | 53.694 | | |
| ATOM | 393 CB | | | | | 1.00 16.86 | AAAA |
| atom | 394 OG | | | | 53.459 | 1.00 24.11 | AAAA |
| ATOM | 395 C | | | | - | | AAAA |
| MOTA | 396 0 | SER 49 | , | | - . | | • |
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| | | | | | 1.50.0.0 | | | | |
|------|-----|------------|------|------|----------|--------|---------|------------|------|
| ATOM | 397 | N | ARG | 50 | 46.890 | 35.805 | 53.519 | 1.00 16.83 | AAAA |
| | 398 | CA | ARG | 50 | 47.724 | 35.037 | 52.610 | 1.00 23.88 | AAAA |
| ATOM | | | _ | 50 | 48.805 | 34.247 | 53.366 | 1.00 27.48 | AAAA |
| ATOM | 399 | CB | ARG | | | | 54.177 | 1.00 22.99 | AAAA |
| ATOM | 400 | CG | ARG | 50 | 48.284 | 33.036 | | 1.00 25.20 | AAAA |
| ATOM | 401 | CD | ARG | 50 | 49.453 | 32.263 | 54.759 | | |
| ATOM | 402 | NE | ARG | 50 | 49.073 | 31.197 | 55.684 | 1.00 15.88 | AAAA |
| ATOM | 403 | CZ | ARG | 50 | 48.411 | 30.093 | 55.368 | 1.00 14.34 | AAAA |
| | 404 | NH1 | | 50 | 48.023 | 29.863 | 54.117 | 1.00 15.78 | AAAA |
| ATOM | | | ARG | . 50 | 48.150 | 29.197 | 56.312 | 1.00 16.78 | AAAA |
| MOTA | 405 | | | | 46.821 | 34.023 | 51.905 | 1.00 20.20 | AAAA |
| ATOM | 406 | C | ARG | 50 | . 45.763 | 33.650 | 52.414 | 1.00 18.63 | AAAA |
| atom | 407 | 0 | ARG | 50 | _ | | 50.699 | 1.00 15.63 | AAAA |
| ATOM | 408 | N | PRO | 51 | 47.203 | 33.596 | | 1.00 13.63 | AAAA |
| ATOM | 409 | CD | PRO | 51 | 48.322 | 34.028 | 49.850 | | |
| ATOM | 410 | CA | PRO | 51 | 46.387 | 32.606 | 49.994 | 1.00 14.35 | AAAA |
| ATOM | 411 | CB | PRO | 51 | 47.076 | 32.514 | 48.629 | 1.00 17.73 | AAAA |
| ATOM | 412 | CG | PRO | 51 | 47.707 | 33.890 | 48.47-5 | 1.00 17.62 | AAAA |
| | 413 | C | PRO | 51 | 46.452 | 31.256 | 50.708 | 1.00 15.73 | AAAA |
| ATOM | | Ö | PRO | 51 | 47.460 | 30.942 | 51.350 | 1.00 18.67 | AAAA |
| ATOM | 414 | | | 52 | 45.377 | 30.470 | 50.618 | 1.00 11.47 | AAAA |
| ATOM | 415 | N | ALA | | 45.375 | 29.117 | 51.161 | 1.00 9.78 | AAAA |
| MOTA | 416 | CA | ALA | 52 | | | 51.112 | 1.00 12.19 | AAAA |
| ATOM | 417 | CB | ALA | 52 | 43.967 | 28.529 | | 1.00 17.19 | AAAA |
| ATOM | 418 | С | ALA | 52 | 46.301 | 28.342 | 50.209 | | |
| MOTA | 419 | 0 | ALA | 52 | 46.307 | 28.609 | 49.006 | 1.00 16.46 | AAAA |
| ATOM | 420 | N | THR | 53 | 47.081 | 27.392 | 50.723 | 1.00 16.40 | AAAA |
| ATOM | 421 | CA | THR | 53 | 47.952 | 26.615 | 49.843 | 1.00 16.32 | AAAA |
| | 422 | CB | THR | 53 | 49.109 | 25.959 | 50.612 | 1.00 15.82 | AAAA |
| ATOM | | OG1 | THR | | 48.582 | 25.016 | 51.559 | 1.00 16.25 | AAAA |
| MOTA | | | | 53 | 49.923 | 27.030 | 51.336 | 1.00 14.34 | AAAA |
| ATOM | 424 | CG2 | THR | | 47.104 | 25.520 | 49.215 | 1.00 14.06 | AAAA |
| MOTA | 425 | C | THR | 53 | 46.012 | 25.241 | 49.690 | 1.00 17.87 | AAAA |
| MOTA | 426 | 0 | THR | 53 | | | 48.145 | 1.00 16.10 | AAAA |
| ATOM | 427 | N | LYS. | 54 | 47.599 | 24.903 | | | AAAA |
| MOTA | 428 | $C\lambda$ | LYS | 54 | 46.848 | 23.832 | 47.492 | 1.00 19.00 | |
| ATOM | 429 | CB | LYS | 54 | 47.671 | 23.245 | 46.339 | 1.00 22.92 | AAAA |
| ATOM | 430 | CG | LYS | 54 | 46.955 | 22.172 | 45.539 | 1.00 32.99 | AAAA |
| ATOM | 431 | CD | LYS | 54 | 45.787 | 22.733 | 44.757 | 1.00 51.34 | AAAA |
| MOTA | 432 | CE | LYS | 54 | 46.244 | 23.565 | 43.561 | 1.00 64.17 | AAAA |
| | 433 | NZ | LYS | 54 | 46.898 | 22.733 | 42.505 | 1.00 63.45 | AAAA |
| atom | | | LYS | 54 | 46.554 | 22.738 | 48.520 | 1.00 22.48 | AAAA |
| ATOM | 434 | C | | 54 | 45.463 | 22.158 | 48.555 | 1.00 19.97 | AAAA |
| Mota | 435 | 0 | LYS | | 47.536 | 22.465 | 49.364 | 1.00 25.65 | AAAA |
| ATOM | 436 | N | GLU | 55 | 47.389 | 21.432 | 50.383 | 1.00 25.08 | AAAA |
| ATOM | 437 | CA | GLU | 55 | 10 710 | | 51.116 | 1.00 25.40 | AAAA |
| ATOM | 438 | CB | GLU | _ | . 48.718 | 21.241 | | 1.00 48.95 | AAAA |
| ATOM | 439 | CG | GLU | 55 | 48.703 | 20.185 | 52.199 | - | AAAA |
| ATOM | 440 | CD | GLU | 55 | 50.106 | 19.821 | 52.673 | 1.00 64.21 | |
| MOTA | 441 | OE1 | GLU | 55 | 50.220 | 19.033 | 53.640 | 1.00 62.38 | AAAA |
| ATOM | 42 | OE2 | GLU | 55 | 51.093 | 20.311 | 52.073 | 1.00 58.22 | AAAA |
| ATOM | .43 | С | GLU | 55 | 46.273 | 21.773 | 51.362 | 1.00 18.91 | AAAA |
| | -44 | ŏ | GLU | 55 | 45.489 | 20.908 | 51.723 | 1.00 17.43 | AAAA |
| ATOM | 445 | N | GLU | 56 | 46.196 | 23.029 | 51.786 | 1.00 16.80 | AAAA |
| ATOM | | | | 56 | 45.137 | 23.432 | 52.698 | 1.00 17.24 | AAAA |
| MOTA | 446 | CA | GLU | | 45.399 | 24.855 | 53.204 | | AAAA |
| MOTA | 447 | CB | GLU | 56 | | | 54.009 | 1.00 14.41 | AAAA |
| ATOM | 448 | CG | GLU | 56 | 46.709 | 24.941 | 54.009 | 1.00 20.17 | AAAA |
| MOTA | 449 | CD | GLU | 56 | 47.087 | 26.354 | 54.358 | | AAAA |
| MOTA | 450 | OE1 | GLU | 56 | 46.713 | 27.252 | | 1.00 17.12 | |
| ATOM | 451 | | GLU | 56 | 47.773 | 26.564 | 55.394 | 1.00 18.23 | AAAA |
| ATOM | 452 | C | GLU | 56 | 43.781 | 23.313 | 52.000 | 1.00 15.95 | AAAA |
| | 453 | ō | GLU | 56 | 42.799 | 22.869 | 52.599 | 1.00 17.82 | AAAA |
| ATOM | | | LEU | 57 | 43.722 | 23.691 | 50.725 | 1.00 17.53 | AAAA |
| ATOM | 454 | N | | 57 | 42.466 | 23.579 | 49.989 | 1.00 16.34 | AAAA |
| ATOM | 455 | CA | LEU | | 42.591 | 24.177 | | 1.00 13.86 | AAAA |
| ATOM | 456 | CB | LEU | 57 | | | | 1.00 15.24 | AAAA |
| ATOM | 457 | CG | LEU | 57 | 42.773 | 25.707 | 40.002 | 1.00 19.30 | AAAA |
| ATOM | 458 | CD1 | LEU | 57 | 42.923 | 26.182 | 47.101 | | AAAA |
| ATOM | 459 | CD2 | LEU | 57 | 41.546 | 26.380 | | 1.00 15.14 | AAAA |
| ATOM | 460 | C | LEU | 57 | 42.016 | | | 1.00 18.46 | |
| ATOM | 461 | ō | LEU | | 40.824 | 21.823 | | | AAAA |
| | 462 | N | LEU | | 42.975 | 21.234 | 49.636 | 1.00 16.43 | AAAA |
| ATOM | 402 | | | | | | • | | • |

| | | | | | 115410100 | | | | |
|------|-----|-----|-----|----|-----------|--------|--------|------------|--------|
| ATOM | 463 | CA | LEU | 58 | 42.662 | 19.822 | 49.475 | 1.00 15.18 | AAAA |
| ATOM | 464 | CB | LEU | 58 | 43.788 | 19.113 | 48.727 | 1.00 16.09 | AAAA |
| ATOM | 465 | CG | LEU | 58 | 44.029 | 19.682 | 47.321 | 1.00 21.72 | AAAA |
| ATOM | 466 | CD1 | LEU | 58 | 45.221 | 18.982 | 46.680 | 1.00 31.92 | AAAA |
| ATOM | 467 | | LEU | 58 | 42.786 | 19.549 | 46.469 | 1.00 34.38 | AAAA |
| ATOM | 468 | C | LEU | 58 | 42.339 | 19.116 | 50.787 | 1.00 21.19 | AAAA |
| ATOM | 469 | ō | LEU | 58 | 42.067 | 17.914 | 50.795 | 1.00 20.40 | AAAA |
| ATOM | 470 | N | LEU | 59 | 42.377 | 19.849 | 51.896 | 1.00 13.50 | AAAA |
| ATOM | 471 | CA | LEU | 59 | 41.958 | 19.261 | 53.173 | 1.00 15.58 | AAAA |
| ATOM | 472 | | LEU | 59 | 42.182 | 20.236 | 54.339 | 1.00 18.98 | AAAA |
| ATOM | 473 | CG | LEU | 59 | 43.619 | | 54.774 | 1.00 22.57 | AAAA |
| ATOM | 474 | | LEU | 59 | 43.640 | 21.654 | 55.808 | 1.00 19.88 | AAAA |
| ATOM | 475 | | LEU | | 44.255 | 19.253 | 55.339 | 1.00 26.71 | AAAA |
| ATOM | 476 | c | LEU | 59 | 40.446 | 18.979 | 53.043 | 1.00 17.55 | AAAA |
| ATOM | 477 | Ö | LEU | 59 | 39.897 | 18.112 | 53.724 | 1.00 18.02 | AAAA |
| MOTA | 478 | N | PHE | 60 | 39.766 | 19.737 | 52.179 | 1.00 14.64 | - AAAA |
| ATOM | 479 | CA | PHE | 60 | 38.338 | 19.536 | 51.970 | 1.00 18.17 | AAAA |
| ATOM | 480 | CB | PHE | 60 | . 37.519 | 20.694 | 52.557 | 1.00 18.80 | AAAA |
| ATOM | 481 | CG | PHE | 60 | 36.028 | 20.564 | 52.316 | 1.00 15.94 | AAAA |
| ATOM | 482 | | PHE | 60 | 35.320 | 19.476 | 52.817 | 1.00 19.98 | AAAA |
| ATOM | 483 | | PHE | 60 | 35.339 | 21.524 | 51.576 | 1.00 18.09 | AAAA |
| ATOM | 484 | | PHE | 60 | 33.947 | 19.338 | 52.587 | 1.00 18.72 | · AAAA |
| ATOM | 485 | | PHE | 60 | 33.964 | 21.399 | 51.338 | 1.00 19.19 | AAAA |
| ATOM | 486 | CZ | PHE | 60 | 33.268 | 20.295 | 51.850 | 1.00 18.43 | AAAA |
| ATOM | 487 | C | PHE | 60 | 37.916 | 19.337 | 50.510 | 1.00 16.45 | AAAA |
| ATOM | 488 | ō | PHE | 60 | 37.227 | 18.371 | 50.179 | 1.00 19.18 | AAAA |
| ATOM | 489 | N | HIS | 61 | 38.308 | 20.257 | 49.638 | 1.00 18.26 | AAAA |
| ATOM | 490 | CA | HIS | | 37.913 | 20.163 | 48.235 | 1.00 14.47 | AAAA |
| ATOM | 491 | CB | HIS | 61 | 38.004 | 21.545 | 47.582 | 1.00 17.15 | AAAA |
| ATOM | 492 | ÇĞ | HIS | 61 | 36.968 | 22.494 | 48.084 | 1.00 14.20 | AAAA |
| ATOM | 493 | | HIS | 61 | 35.645 | 22.580 | 47.816 | 1.00 11.05 | AAAA |
| ATOM | 494 | | HIS | 61 | 37.237 | 23.477 | 49.012 | 1.00 23.25 | AAAA |
| ATOM | 495 | | HIS | 61 | 36.121 | 24.131 | 49.291 | 1.00 13.35 | AAA:A |
| ATOM | 496 | | HIS | 61 | 35.143 | 23.606 | 48.579 | 1.00 21.07 | AAAA |
| ATOM | 497 | С | HIS | 61 | 38.695 | 19.157 | 47.417 | 1.00 18.29 | AAAA |
| ATOM | 498 | 0 | HIS | 61 | 39.828 | 18.819 | 47.761 | 1.00 17.50 | AAAA |
| ATOM | 499 | N | THR | 62 | 38.071 | 18.658 | 46.346 | 1.00 15.39 | AAAA |
| ATOM | 500 | CA | THR | 62 | 38.741 | 17.686 | 45.473 | 1.00 19.02 | AAAA |
| MOTA | 501 | CB | THR | 62 | 37.734 | 16.767 | 44.756 | 1.00 19.61 | AAAA |
| ATOM | 502 | OG1 | THR | 62 | 36.795 | 17.548 | 44.006 | 1.00 22.05 | AAAA |
| ATOM | 503 | CG2 | THR | 62 | 36.995 | 15.925 | 45.767 | 1.00 28.99 | AAAA |
| MOTA | 504 | С | THR | 62 | 39.595 | 18.398 | 44.440 | 1.00 23.22 | AAAA |
| ATOM | 505 | 0 | THR | 62 | 39.311 | 19.532 | 44.044 | 1.00 17.47 | AAAA |
| ATOM | 506 | IJ | GLU | 63 | 40.657 | 17.732 | 44.009 | 1.00 18.94 | AAAA |
| ATOM | 507 | CA | GLU | 63 | 41.571 | 18.324 | 43.046 | 1.00 22.44 | AAAA |
| ATOM | 508 | CB | GLU | 63 | 42.736 | | | 1.00 28.31 | AAAA |
| ATOM | 509 | CG | GLU | 63 | 43.885 | 17.476 | 43.708 | 1.00 60.37 | AAAA |
| ATOM | 510 | CD | GLU | 63 | 45.154 | 16.893 | 43.115 | 1.00 65.08 | AAAA |
| ATOM | 511 | | GLU | 63 | 45.603 | 17.407 | 42.065 | 1.00 66.44 | AAAA |
| ATOM | 512 | OE2 | GLU | 63 | 45.697 | 15.927 | 43.694 | 1.00 71.72 | AAAA |
| ATOM | 513 | С | GLU | 63 | 40.983 | 18.764 | 41.730 | 1.00 18.63 | AAAA |
| ATOM | 514 | 0 | GLU | 63 | 41.340 | 19.827 | 41.228 | 1.00 18.37 | AAAA |
| ATOM | 515 | N | ASP | 64 | 40.108 | 17.943 | 41.153 | 1.00 19.77 | AAAA |
| ATOM | 515 | CA | ASP | 64 | 39.508 | 18.277 | 39.864 | 1.00 17.88 | AAAA |
| MOTA | 517 | CB | ASP | 64 | 38.584 | 17.159 | 39.372 | 1.00 20.43 | AAAA |
| ATOM | 518 | CG | ASP | 64 | 37.429 | 16.884 | 40.330 | 1.00 42.71 | AAAA |
| ATOM | 519 | | ASP | 64 | 36.415 | 16.291 | 39.899 | 1.00 45.01 | AAAA |
| ATOM | 520 | | asp | 64 | 37.537 | 17.243 | 41.521 | 1.00 51.77 | AAAA |
| ATOM | 521 | С | ASP | 64 | 38.701 | 19.582 | 39.964 | 1.00 21.90 | АААА |
| ATOM | 522 | O | ASP | 64 | 38.726 | 20.410 | 39.042 | 1.00 17.35 | AAAA |
| ATOM | 523 | N | TYR | 65 | 37.980 | 19.750 | 41.072 | 1.00 16.17 | AAAA |
| ATOM | 524 | CA | TYR | 65 | 37.178 | 20.957 | 41.292 | 1.00 15.62 | AAAA |
| ATOM | 525 | CB | TYR | 65 | 36.258 | 20.796 | 42.529 | 1.00 12.04 | AAAA |
| ATOM | 526 | CG | TYR | 65 | 35.501 | 22.065 | 42.886 | 1.00 12.23 | AAAA |
| ATOM | 527 | | TYR | 65 | 34.699 | 22.718 | 41.940 | 1.00 14.73 | AAAA |
| ATOM | 528 | CE1 | TYR | 65 | 34.028 | 23.910 | 42.253 | 1.00 18.23 | AAAA |

| ATOM | 529 | CD2 | TYR | 65 | 35.609 | 22.631 | 44.163 | 1.00 13.67 | AAAA |
|--------|-------|-----|------|----|--------|--------|--------|------------|--------|
| | - | | | | 34.943 | 23.824 | 44.486 | 1.00 18.16 | AAAA |
| ATOM | 530 | CE2 | TYR | 65 | | | | | |
| MOTA | 531 | CZ | TYR | 65 | 34.162 | 24.461 | 43.533 | 1.00 16.88 | AAAA |
| | | | | | 33.555 | 25.665 | 43.837 | 1.00 14.59 | AAAA |
| ATOM | 532 | OH | TYR | 65 | | | | | |
| MOTA | 533 | С | TYR | 65 | 38.090 | 22.177 | 41.459 | 1.00 15.27 | AAAA |
| | | | | | 37.882 | 23.189 | 40.798 | 1.00 15.96 | AAAA |
| ATOM | 534 | 0 | TYR | 65 | | | | | |
| ATOM | 535 | N | ILE | 66 | 39.098 | 22.073 | 42.321 | 1.00 14.29 | AAAA |
| | | | | | 40.022 | 23.179 | 42.540 | 1.00 18.86 | AAAA |
| MOTA | 536 | CA | ILE | 66 | | | | | |
| ATOM | 537 | CB | ILE | 66 | 41.090 | 22.836 | 43.617 | 1.00 15.56 | AAAA |
| | | | | | 42.152 | 23.943 | 43.698 | 1.00 20.45 | AAAA |
| ATOM | 538 | CG2 | | 66 | | | | | |
| ATOM | 539 | CG1 | TIE | 66 | 40.405 | 22.659 | 44.967 | 1.00 19.68 | AAAA |
| | | | | | 39.717 | 23.948 | 45.454 | 1.00 29.11 | AAAA |
| MOTA | 540 | CD1 | 1112 | 66 | | | | | |
| MOTA | 541 | С | ILE | 66 | 40.716 | 23.519 | 41.236 | 1.00 25.20 | AAAA |
| | | | | | 40.809 | 24.692 | 40.895 | 1.00 14.60 | AAAA |
| ATOM | 542 | 0 | ILE | 66 | 40.603 | | | | |
| ATOM | 543 | N | ASN | 67 | 41.190 | 22.508 | 40.498 | 1.00 18.21 | AAAA |
| | | | | | 41.879 | 22.789 | 39.236 | 1.00 20.03 | AAAA |
| MOTA | 544 | CA | ASN | 67 | | | | | |
| ATOM | 545 | CB | ASN | 67 | 42.448 | 21.523 | 38.580 | 1.00 21.73 | AAAA |
| | - | | | | 43.645 | 20.954 | 39.333 | 1.00 21.69 | AAAA |
| ATOM | 546 | CG | ASN | 67 | | | | | |
| ATOM | 547 | OD1 | 2SN | 67 | 44.293 | 21.645 | 40.110 | 1.00 23.97 | AAAA |
| | | | | 67 | 43.947 | 19.692 | 39.086 | 1.00 23.23 | AAAA |
| ATOM | 548 | ND2 | | | | | | | |
| ATOM | 549 | С | ASN | 67 | 40.970 | 23.500 | 38.250 | 1.00 15.87 | AAAA |
| | | | | 67 | 41.431 | 24.347 | 37.473 | 1.00 18.64 | AAAA |
| ATOM | 550 | 0 | ASN | | | | | | |
| ATOM | 551 | N | THR | 68 | 39.681 | 23.180 | 38.295 | 1.00 16.55 | AAAA |
| | | | | 68 | 38.729 | 23.814 | 37.400 | 1.00 20.34 | AAAA |
| ATOM | 552 | CA | THR | | | | | | |
| ATOM | 553 | CB | THR | 68 | 37.360 | 23.114 | 37.441 | 1.00 22.99 | AAAA |
| | | | | 68 | 37.511 | 21.760 | 36.978 | 1.00 21.75 | AAAA |
| ATOM | 554 | OG1 | | | | | | | |
| ATOM | 555 | CG2 | THR | 68 | 36.378 | 23.827 | 36.536 | 1.00 17.37 | AAAA |
| | | | | | 38.561 | 25.291 | 37.755 | 1.00 16.66 | AAAA |
| ATOM | 556 | С | THR | 68 | | | | | AAAA |
| ATOM | 557 | 0 | THR | 68 | 38.472 | 26.139 | 36.871 | 1.00 18.79 | |
| | | | LEU | 69 | 38.534 | 25.604 | 39.045 | 1.00 14.82 | AAAA |
| ATOM | 558 | N | | | | | | | AAAA |
| ATOM | 559 | CA | LEU | 69 | 38.405 | 27.000 | 39.447 | 1.00 15.20 | |
| | 560 | CB | LEU | 69 | 38.295 | 27.126 | 40.973 | 1.00 16.87 | AAAA · |
| MOTA | | | | | | | | 1.00 14.76 | AAAA |
| MOTA | 561 | CG | LEU | 69 | 37.057 | 26.551 | 41.666 | | |
| | 562 | CDI | LEU | 69 | 37.212 | 26.643 | 43.179 | 1.00 16.81 | AAAA |
| MOTA | | | | | | | | 1.00 17.26 | AAAA |
| ATOM | 563 | CD2 | LEU | 69 | 35.832 | 27.312 | 41.217 | | |
| | 564 | С | LEU | 69 | 39.623 | 27.796 | 38.969 | 1.00 15.11 | AAAA |
| MOTA | | | | | | 28.934 | 38.504 | 1.00 13.30 | AAAA |
| ATOM | 565 | 0 | LEU | 69 | 39.500 | | | | |
| MOTA | 566 | N | MET | 70 | 40.803 | 27.204 | 39.090 | 1.00 13.40 | AAAA |
| | | | | | 42.019 | 27.894 | 38.659 | 1.00 16.97 | AAAA |
| ATOM | 567 | CA | MET | 70 | | | | | |
| ATOM | . 568 | CB | MET | 70 | 43.254 | 27.114 | 39.075 | 1.00 14.87 | AAAA |
| | | | | | 43.335 | 26.886 | 40.582 | 1.00 15.18 | AAAA |
| ATOM | 569 | CG | MET | 70 | | | | | |
| MOTA | 570 | SD | ET | 70 | 44.828 | 25.954 | 41.060 | 1.00 28.71 | AAAA |
| | | | | 70 | 46.051 | 27.228 | 40.893 | 1.00 21.19 | AAAA |
| ATOM | 571 | CE | MET | | | | | | |
| ATOM | 572 | С | MET | 70 | 42.064 | 28.119 | 37.155 | 1.00 19.11 | AAAA |
| | | | | 70 | 42.498 | 29.170 | 36.700 | 1.00 17.10 | AAAA |
| MOTA | 573 | 0 | MET | | | | | | AAAA |
| MOTA | . 574 | N | GL! | 71 | 41.648 | 27.118 | 36.389 | 1.00 15.06 | |
| | | | GLU | 71 | 41.651 | 27.226 | 34.934 | 1.00 16.12 | AAAA |
| ATOM | 575 | CA | | | | | | 1 00 16 12 | AAAA |
| ATOM | 576 | CB | GLi | 71 | 41.397 | 25.856 | 34.305 | 1.00 16.12 | |
| | 577 | CG | GLU | 71 | 41.387 | 25.882 | 32.800 | 1.00 20.26 | AAAA |
| ATOM | | | | | | | | 1.00 32.31 | AAAA |
| ATOM | 578 | CD | GLU | 71 | 42.782 | 25.920 | 32.193 | | |
| | 579 | OFI | GLU | 71 | 42.893 | 25.741 | 30.958 | 1.00 27.07 | AAAA |
| ATOM | | | | | | | 32.941 | 1.00 24.85 | AAAA |
| ATOM | 580 | OE2 | 3LU | 71 | 43.762 | 26.117 | | | |
| ATOM | 581 | С | GLU | 71 | 40.580 | 28.208 | 34.466 | 1.00 16.48 | AAAA |
| | | | | | | 29.066 | 33.611 | 1.00 17.20 | AAAA |
| ATOM | - 582 | 0 | GLU | 71 | 40.831 | | | | |
| ATOM | 583 | N | ALA | 72 | 39.380 | 28.097 | 35.027 | 1.00 15.68 | AAAA |
| | | | | | | | 34.644 | 1.00 16.07 | AAAA |
| ATOM | 584 | CA | ALA | 72 | 38.300 | 28.998 | | | |
| | 585 | CB | ALA | 72 | 37.035 | 28.669 | 35.425 | 1.00 17.21 | AAAA |
| ATOM | | | | | | 30.453 | 34.897 | 1.00 19.07 | AAAA |
| MOTA | 586 | C | ALA | 72 | 38.678 | | | | |
| | 587 | 0 | ALA | 72 | 38.448 | 31.326 | 34.054 | 1.00 15.92 | AAAA |
| ATOM | | | | | | | 36.062 | 1.00 15.86 | AAAA |
| ATOM | 588 | N | GLU | 73 | 39.260 | 30.726 | | | |
| | | | GLU | 73 | 39.616 | 32.097 | 36.372 | 1.00 15.50 | AAAA |
| MOTA | 589 | CA | | | | | | 1.00 14.12 | AAAA |
| ATOM | 590 | CB | GLU | 73 | 40.046 | 32.210 | 37.828 | | |
| | | | | 73 | 40.430 | 33.615 | 38.214 | 1.00 14.24 | AAAA |
| atom | 591 | CG | GLU | | | | | 1.00 17.23 | AAAA |
| ATOM | 592 | CD | GLU | 73 | 40.961 | 33.699 | 39.629 | 1.00 17.23 | |
| | | | | 73 | 40.147 | 33.696 | 40.573 | 1.00 18.51 | AAAA |
| ATOM | 593 | | GLU | | | | | 1.00 20.88 | AAAA |
| ATOM | 594 | OE2 | GLU | 73 | 42.201 | 33.753 | 39.793 | 1.00 20.00 | Anna |
| 21.012 | | | | | | | - | | • |
| | | | | | | | | | |

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|--------------|------------|-----------|------------|------------|--------|--------|--------|--------------------------|--------------|
| | 595 | С | GLU | 73 | 40.706 | 32.709 | 35.495 | 1.00 20.36 | AAAA |
| MOTA | 596 | Ö | GLU | 73 | 40.527 | 33.806 | 34.948 | 1.00 17.74 | AAAA |
| ATOM | | | ARG | 74 | 41.832 | 32.020 | 35.344 | 1.00 21.57 | AAAA |
| MOTA | 597 | N | ARG | 74 | 42.911 | 32.623 | 34.574 | 1.00 19.48 | AAAA |
| MOTA | 598 | CA | ARG | 74 | 44.256 | 31.912 | 34.834 | 1.00 18.48 | AAAA |
| MOTA | 599 | CB | | 74 | 44.365 | 30.489 | 34.351 | 1.00 14.96 | AAAA |
| MOTA | 600 | CG | ARG | 74 | 45.723 | 29.892 | 34.745 | 1.00 15.05 | AAAA |
| MOTA | 601 | CD | ARG | 74 | 45.918 | 28.696 | 33.950 | 1.00 18.16 | AAAA |
| MOTA | 602 | NE | ARG | . 74 | 46.439 | 28.682 | 32.727 | 1.00 16.31 | AAAA |
| ATOM | 603 | CZ | ARG | | 46.843 | 29.811 | 32.145 | 1.00 19.74 | AAAA |
| ATOM | 604 | | ARG | 74 | 46.466 | 27.536 | 32.047 | 1.00 14.73 | AAAA |
| ATOM | 605 | | ARG | 74 | 42.643 | 32.718 | 33.084 | 1.00 16.86 | AAAA |
| MOTA | 606 | C | ARG | 74 | 43.148 | 33.621 | 32.426 | 1.00 15.41 | AAAA |
| MOTA | 607 | 0 | ARG | 74 · 75 | 41.859 | 31.794 | 32.547 | 1.00 17.56 | AAAA |
| ATOM | 608 | N | CYS | 75 75 | 41.544 | 31.833 | 31.115 | 1.00 18.24 | AAAA |
| MOTA | 609 | CA | CYS | 75 75 | 41.474 | 30.414 | 30.545 | 1.00 20.94 | AAAA |
| MOTA | 610 | CB | CYS | 75 75 | 43.047 | 29.514 | 30.572 | 1.00 19.30 | AAAA |
| MOTA | 611 | SG | CÝS | 75 75 | 40.216 | 32.561 | 30.898 | 1.00 15.81 | AAAA |
| MOTA | 612 | С | CYS | 75 75 | 39.762 | 32.748 | 29.762 | 1.00 17.79 | AAAA |
| MOTA | 613 | 0 | CYS | 75 76 | 39.601 | 32.959 | 32.007 | 1.00 15.63· | AAAA - |
| MOTA | 614 | N | GLN | | 38.339 | 33.686 | 32.010 | 1.00 23.22 | AAAA |
| ATOM | 615 | CA | GLN | 76 76 | 38.595 | 35.122 | 31.530 | 1.00 22.99 | AAAA |
| A·I·OM | 616 | CB | GLN | 76 76 | 37.564 | 36.107 | 32.027 | 1.00 44.69 | AAAA |
| ATOM | 617 | CG | GLN | 76 76 | 37.588 | 36.229 | 33.535 | 1.00 47.78 | AAAA |
| MOTA | 618 | CD | GLN | 76 76 | 37.563 | 35.228 | 34.243 | 1.00 62.95 | AAAA |
| ATOM | 619 | | GLN | 76 76 | 37.619 | 37.452 | 34.033 | 1.00 45.96 | AAAA |
| MOTA | 620 | NE2 | | 76 76 | 37.304 | 32.975 | 31.135 | 1.00 23.43 | AAAA |
| MOTA | 621 | С | GLN | 76 76 | 36.826 | 33.512 | 30.135 | 1.00 19.93 | AAAA |
| MOTA | 622 | 0 | GLN | 76 77 | 36.951 | 31.754 | 31.521 | 1.00 15.97 | AAAA |
| ATOM | 623 | N | CYS | 77 77 | 36.004 | 30.979 | 30.741 | 1.00 18.91 | AAAA |
| MOTA | 624 | CA | CYS | 77 | 36.738 | 30.225 | 29.623 | 1.00 24.64 | AAAA |
| MOTA | 625 | CB | CYS | 77 | 37.848 | 28.887 | 30.269 | 1.00 25.26 | AAAA |
| ATOM | 626 | SG | CYS | 77 | 35.302 | 29.951 | 31.594 | 1.00 19.68 | AAAA |
| MOTA | 627 | C | CYS | 77 | 35.685 | 29.702 | 32.732 | 1.00 20.02 | AAAA |
| MOTA | 628 | 0 | CYS | 78 | 34.254 | 29.366 | 31.022 | 1.00 16.00 | AAAA |
| MOTA | 629 | N | VAL VAL | 78 | 33.531 | 28.288 | 31.671 | 1.00 18.73 | AAAA |
| MOTA | 630 | CA | VAL | 78 78 | 32.016 | 28.455 | 31.557 | 1.00 15.57 | AAAA |
| ATOM | 631 632 | CB CC1 | VAL | 78 | 31.312 | 27.304 | 32.262 | 1.00 21.27 | AAAA |
| ATOM | 633 | | VAL | 78 | 31.603 | 29.792 | 32.151 | 1.00 19.47 | AAAA |
| ATOM | 634 | C | VAL | 78 | 33.950 | 27.077 | 30.859 | 1.00 24.02 | AAAA |
| ATOM | 635 | Ö | VAL | 78 | 33.499 | 26.894 | 29.718 | 1.00 24.08 | AAAA |
| ATOM | 636 | N | PRO | 79 | 34.848 | 26.249 | 31.420 | 1.00 18.91 | AAAA AAAA |
| MOTA MOTA | 637 | CD | PRO | 79 | 35.470 | 26.341 | 32.756 | 1.00 17.70 | AAAA |
| ATOM | 638 | CA | PRO | 79 | 35.320 | 25.056 | 30.720 | 1.00 23.37 | AAAA |
| | 639 | СВ | PRO | 79 | 36.295 | 24.432 | 31.732 | 1.00 21.92 | AAA. |
| MOTA ATOM | 640 | CG | PRO | 79 | 36.802 | 25.677 | | 1.00 20.90 | AAA. |
| MOTA | 641 | c | PRO | 79 | 34.152 | 24.144 | | 1.00 27.44 | AAA |
| MOTA | 642 | 0 | PRO | 79 | 33.177 | | | 1.00 22.20 1.00 23.35 | AAAA |
| MOTA | 643 | N | LYS | 80 | 34.245 | | | | AAAA |
| ATOM | 644 | CA | LYS | 80 | 33.212 | | | 1.00 20.70 | AAAA |
| MOTA | 645 | CB | LYS | 80 | 33.708 | | | 1.00 52.33 | AAAA |
| ATOM | 646 | CG | LYS | 80 | 35.098 | | | 1.00 68.70 | AAAA |
| MOTA | 647 | CD | LYS | 80 | 35.669 | | | 1.00 70.04 | AAAA |
| MOTA | 648 | CE | LYS | 80 | 37.131 | | | 1.00 73.72 | AAAA |
| ATOM | 649 | NZ | LYS | 80 | 37.688 | | | | AAAA |
| ATOM | 650 | С | LYS | 80 | 32.875 | 21.571 | | | AAAA |
| MOTA | 651 | ၁ | LYS | 80 | 33.770 | | | 1 | AAAA |
| ATOM | 652 | N | GLY | 81 | 31.582 | | | | AAAA |
| MOTA | 653 | | | 81 | 31.126 | 20.509 | | | AAAA |
| ATOM | 654 | | GLY | 81 | 31.151 | 21.039 | | | AAAA |
| ATOM | 655 | | GLY | 81 | 30.604 | | | | AAAA |
| ATOM | 656 | | ALA | 82 | 31.754 | | | | AAAA |
| ATOM | 657 | | | 82 | 31.858 | 22.738 | | | AAAA |
| ATOM | 658 | | | 82 | 33.065 | | | | AAAA |
| ATCM | 659 | | ALA | 82 | 30.610 | | | | AAAA |
| ATCM | 660 | | ALA | 82 | 30.425 | 23.529 | מוני ק | . 1.00 20.00 | • |
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| | | | | • | | | | | |
|------|-----|-----|----------------------|-----------|-----------------|--------|--------|------------|---------------|
| ATOM | 661 | N | ARG | 83 | 29.758 | 23.926 | 33.897 | 1.00 17.68 | AAAA |
| | | CA | AEG | 83 | 28.549 | 24.596 | 34.360 | 1.00 15.04 | AAAA |
| ATCM | 662 | | | | | | 33.176 | 1.00 21.02 | AAAA |
| ATCM | 663 | CB | ARG | 83 | 27.777 | 25.188 | | | |
| ATCM | 664 | CG | ARG | 83 | 26.938 | 26.395 | 33.528 | 1.00 36.77 | AAAA |
| ATCM | 665 | CD | ARG | 83 | 26.061 | 26.167 | 34.729 | 1.00 41.28 | AAAA |
| ATCM | 666 | NE | ARG | 83 | 25.366 | 27.393 | 35.105 | 1.00 40.05 | AAAA |
| | | | ARG | 83 | 24.530 | 27.492 | 36.134 | 1.00 51.15 | AAAA |
| ATCM | 667 | | | | | | 36.893 | 1.00 55.10 | AAAA |
| MOTA | 668 | | ARG | 83 | 24.286 | 26.432 | | | |
| ATCM | 669 | NH2 | ARG | 83 | 23.931 | 28.646 | 36.399 | 1.00 54.26 | AAAA |
| ATCM | 670 | С | ARG | 83 | 27.701 | 23.530 | 35.030 | 1.00 21.33 | AAAA |
| ATCM | 671 | 0 | ARG | 83 - | 27.193 | 23.708 | 36.130 | 1.00 24.88 | AAAA |
| | 672 | N | GLU | 84 | 27.565 | 22.406 | 34.352 | 1.00 18.76 | AAAA |
| ATOM | | | | 84 | 26.768 | 21.299 | 34.859 | 1.00 24.12 | AAAA |
| MOTA | 673 | CA | GLU | | | | 33.744 | 1.00 32.64 | AAAA |
| ATCM | 674 | CB | GLU | 84 | 26.527 | 20.290 | | | |
| MOTA | 675 | CG | GLU | 84 | 2 7 .769 | 19.994 | 32.925 | 1.00 37.91 | AAAA |
| ATOM | 676 | CD | GLU' | 84 | 27.832 | 20.784 | 31.612 | 1.00 51.24 | AAAA |
| ATOM | 677 | | GLU | 84 | 27.585 | 20.152 | 30.545 | 1.00 24.82 | AAAA |
| | 678 | | GLU | 84 | 28.114 | 22.018 | 31.650 | 1.00 22.57 | AAAA |
| ATCM | | | | | 27.394 | 20.570 | 36.043 | 1.00 25.36 | AAAA |
| MOTA | 679 | С | GLU | 84 | | | | 1.00 26.17 | AAAA |
| MOTA | 680 | 0 | GLU | 84 | 26.739 | 20.321 | 37.057 | | |
| ATCM | 681 | N | LYS | 85 | 28.665 | 20.232 | 35.897 | 1.00 18.78 | AAAA |
| ATOM | 682 | CA | LYS | 85 | 29.399 | 19.497 | 36.915 | 1.00 20.03 | AAAA |
| ATCM | 683 | CB | LYS | 85 | 30.658 | 18.900 | 36.280 | 1.00 18.59 | AAAA |
| | 684 | CG | LYS | 85 | 31.603 | 18.223 | 37.268 | 1.00 35.69 | AAAA |
| ATCM | | | | | 31.151 | 16.832 | 37.644 | 1.00 51.51 | AAAA |
| MOTA | 685 | CD | LYS | 85 | | | | 1.00 59.18 | AAAA |
| ATOM | 686 | CE | LYS | 85 | 31.451 | 15.864 | 36.520 | | AAAA |
| MOTA | 687 | NZ | LYS | 85 | 32.914 | 15.858 | 36.240 | 1.00 56.63 | |
| ATOM | 688 | С | LYS | 85 | 29.811 | 20.263 | 38.181 | 1.00 18.31 | AAAA |
| MOTA | 689 | 0 | LYS | 85 | 29.696 | 19.738 | 39.290 | 1.00 21.65 | AAAA , |
| ATOM | 690 | N | TYR | 86 | 30.274 | 21.495 | 38.012 | 1.00 19.45 | AAAA |
| | 691 | CA | TYR | | 30.776 | 22.272 | 39.145 | 1.00 14.26 | AAAA |
| ATOM | | | | 86 | 32.207 | 22.692 | 38.840 | 1.00 14.95 | AAAA |
| MOTA | 692 | CB | TYR | | | | 38.585 | 1.00 19.76 | AAAA |
| ATCM | 693 | CG | TYR | 86 | 33.107 | 21.508 | | | AAAA |
| MOTA | 694 | CD1 | TYR | 86 . | 33.384 | 20.591 | 39.601 | 1.00 18.83 | |
| ATOM | 695 | CE1 | TYR | 86 | 34.247 | 19.519 | 39.388 | 1.00 20.29 | AAAA |
| ATCM | 696 | CD2 | TYR | 86 | 33.711 | 21.322 | 37.337 | 1.00 18.14 | AAAA |
| ATOM | 697 | | TYR | 86 | 34.567 | 20.261 | 37.112 | 1.00 22.66 | AAAA |
| | | | TYR | 86 | 34.832 | 19.364 | 38.145 | 1.00 22.51 | AAAA |
| MOTA | 698 | CZ | | | | 18.317 | 37.921 | 1.00 23.68 | AAAA |
| MOTA | 699 | ОН | TYR | 86 | 35.680 | | | 1.00 19.03 | AAAA |
| ATOM | 700 | С | TYR | 86 | 29.967 | 23.493 | 39.526 | | |
| ATOM | 701 | 0 | TYR | 86 | 30.353 | 24.226 | 40.450 | 1.00 19.18 | AAAA |
| ATOM | 702 | N | ASN | 87 | 28.873 | 23.721 | 38.803 | 1.00 17.59 | AAAA |
| ATOM | 703 | CA | ASN | 67 | 27.953 | 24.843 | 39.071 | 1.00 18.07 | አአ አ ፉ |
| ATCM | 704 | CB | ASN | 87 | 27.413 | 24.730 | 40.514 | 1.00 23.87 | AAAA |
| | 705 | CG | ASN | 87 | 26.020 | 25.349 | 40.688 | 1.00 30.67 | AAAA |
| ATOM | | | | | 25.531 | 25.520 | 41.819 | 1.00 31.55 | AAAA |
| ATOM | 706 | | ASN | 87 | | | | 1.00 20.18 | AAAA |
| ATOM | 707 | | ASN | 87 | 25.370 | 25.661 | 39.580 | | AAAA |
| ATOM | 708 | C | ASN | 87 | 28.641 | 26.197 | 38.875 | 1.00 24.24 | |
| ATOM | 709 | 0 | ASN | 87 | 28.283 | 27.190 | 39.519 | 1.00 18.57 | AAAA |
| ATCM | 710 | N | ILE | 88 | 29.617 | 26.237 | 37,970 | 1.00 18.80 | AAAA |
| | 711 | CA | ILE | 88 | 30.353 | 27.471 | 37.680 | 1.00 18.55 | AAAA |
| ATCM | | | | | 31.865 | 27.166 | 37.508 | 1.00 26.44 | AAAA |
| ATOM | 712 | CB | ILE | 88 | | | | 1.00 43.71 | AAAA |
| ATOM | 713 | CG2 | ILE | 88 | 32.613 | 28.406 | 37.044 | | |
| MOTA | 714 | CG1 | ILE | 88 | 32.439 | 26.703 | | 1.00 36.30 | AAAA |
| ATOM | 715 | CD1 | | 88 | 32.295 | 27.735 | 39.888 | 1.00 24.08 | AAAA |
| | 716 | c | ILE | 88 | 29.887 | 28.142 | 36.392 | 1.00 14.36 | AAAA |
| ATOM | | | | 38 | 29.584 | 27.459 | 35.426 | 1.00 21.93 | AAAA |
| ATOM | 717 | 0 | ILE | | | | 36.380 | 1.00 18.71 | AAAA |
| ATCM | 718 | N | GLY | 89 | 29.843 | 29.473 | | | AAAA |
| MOTA | 719 | CA | GLY | 89 | 29.479 | 30.162 | 35.154 | 1.00 20.23 | |
| ATCM | 720 | С | GLY | 89 | 28.147 | 30.873 | 35.106 | 1.00 20.85 | AAAA |
| ATOM | 721 | ō | GLY | 89 | 28.006 | 31.817 | 34.330 | 1.00 25.47 | AAAA |
| | 722 | N | GLY | 90 | 27.172 | 30.414 | 35.889 | 1.00 21.17 | AAAA |
| ATOM | | | | 90 | 25.863 | 31.060 | 35.898 | 1.00 24.44 | AAAA |
| ATOM | 723 | CA | GLY | | | | 36.668 | 1.00 30.60 | AAAA |
| ATCM | 724 | С | GLY | 90 | 25.862 | 32.371 | | 1 00 20 13 | AAAA |
| ATCM | 725 | 0 | GLY | 90 | 26.900 | 32.788 | 37.168 | 1.00 28.13 | |
| ATCM | 726 | N | TYR | 91 | 24.708 | 33.036 | 36.755 | 1.00 23.38 | AAAA |
| | | | | | | | - | | |

| | | | | _ | | | | | |
|-------|-----|----------|---------------------|------|--------|--------|---------|------------|--------|
| | | <i>~</i> | TYR | 91 | 24.598 | 34.299 | 37.490 | 1.00 28.48 | AAAA |
| MOTA | 727 | | | | 23.144 | 34.753 | 37.545 | 1.00 29.88 | · AAAA |
| MOTA | 728 | CB | TYR | 91 | | | | 1.00 33.88 | AAAA |
| MOTA | 729 | CG · | TYR | 91 | 22.923 | 35.899 | 38.518 | | |
| | 730 | | TYR | 91 | 23.329 | 37.197 | 38.207 | 1.00 39.69 | AAAA |
| MOTA | | | | | 23.130 | 38.250 | 39.104 | 1.00 31.76 | AAAA |
| MOTA | 731 | | TYR | 91 | 25.150 | | 39.759 | 1.00 40.63 | AAAA |
| ATOM- | 732 | CD2 | TYR | 91 | 22.317 | 35.678 | | 1.00 40.03 | AAAA |
| | 733 | | TYR | 91 | 22.115 | 36.720 | 40.664 | 1.00 37.07 | |
| atom | | | | 91 | 22.521 | 38.002 | 40.327 | 1.00 36.22 | AAAA |
| MOTA | 734 | | TYR | | _ | | 41.210 | 1.00 44.71 | AAAA |
| ATOM | 735 | OH | TYR | 91 | 22.306 | 39.035 | | | AAAA |
| | 736 | C . | TYR | 91 | 25.075 | 34.157 | 38.937 | 1.00 23.59 | |
| ATOM | | _ | | 91 | 25.713 | 35.041 | 39.502 | 1.00 22.64 | AAAA |
| MOTA | 737 | | TYR | | | | 39.531 | 1.00 23.09 | AAAA |
| ATOM | 738 | N | GLU | 92 | 24.724 | 33.032 | | 1.00 25.05 | AAAA |
| | 739 | | GLU | 92 . | 25.048 | 32.747 | 40.917 | 1.00 26.61 | |
| MOTA | | | | 92 | 24.289 | 31.476 | 41.306 | 1.00 32.57 | AAAA |
| ATOM | 740 | | GLU | | | 30.892 | 42.657 | 1.00 41.38 | AAAA |
| ATOM | 741 | CG | GLU | 92 | 24.595 | | - | | - AAAA |
| | 742 | | GLU | 92 | 23.604 | 29.800 | 43.023 | 1.00 49.02 | |
| MOTA | | | | 92 | 24.008 | 28.829 | 43.715 | 1.00 45.51 | AAAA |
| ATOM | 743 | OE1 | | | | | 42.628 | 1.00 38.16 | AAAA |
| ATOM | 744 | OE2 | GLU | 92 | 22.418 | 29.931 | | 1.00 25.78 | AAAA |
| | 745 | C | GLU | 92 | 26.541 | 32.636 | 41.251 | | |
| MOTA | | | | 92 | 27.045 | 33.358 | 42.125 | 1.00 24.95 | AAAA |
| MOTA | 746 | 0 | GLU | | - | 31.742 | 40.556 | 1.00 21.41 | AAAA |
| ATOM | 747 | N | ASN | 93 | 27.243 | | | 1.00 21.14 | AAAA |
| MOTA | 748 | CA | ASN | 93 | 28.674 | 31.519 | 40.777 | 1.00 21.14 | |
| | | | ASN | 93 | 28.876 | 30.075 | 41.226 | 1.00 17.27 | AAAA |
| MOTA | 749 | CB | | | 27.905 | 29.682 | 42.320 | 1.00 15.34 | AAAA |
| MOTA | 750 | CG | ASN | 93 | | | 43.399 | 1.00 20.33 | AAAA |
| ATOM | 751 | OD1 | ASN | 93 | 27.882 | 30.290 | | | AAAA . |
| | 752 | ND2 | | 93 | 27.078 | 28.674 | 42.047 | 1.00 20.49 | |
| MOTA | | | | | 29.378 | 31.778 | 39.445 | 1.00 22.25 | AAAA |
| ATOM | 753 | C | asn | 93 | | | 38.806 | 1.00 20.29 | AAAA |
| MOTA | 754 | 0 | ASN | 93 | 29.901 | 30.865 | | 1.00 25.45 | AAAA |
| | 755 | N· | PRO | 94 | 29.451 | 33.057 | 39.045 | | |
| ATOM | | | PRO | 94 | 29.027 | 34.221 | 39.839 | 1.00 23.03 | AAAA |
| MOTA | 756 | CD | | | 30.055 | 33.523 | 37.794 | 1.00 23.05 | AAAA |
| MOTA | 757 | CA | PRO | 94 | - | | _ | 1.00 28.71 | AAAA |
| ATOM | 758 | CB | PRO | 94 | 29.669 | 35.004 | 37.759 | | AAAA |
| | 759 | CG | PRO | 94 | 28.528 | 35.112 | 38.755 | 1.00 40.02 | |
| MOTA | | | | _ | 31.554 | 33.384 | 37.697 | 1.00 26.51 | AAAA |
| ATOM | 760 | С | PRO | 94 | | 33.185 | 38.688 | 1.00 17.36 | AAAA |
| MOTA | 761 | 0 | PRO | 94 | 32.232 | | | 1.00 21.12 | AAAA |
| | 762 | N | VAL | 95 | 32.068 | 33.498 | 36.478 | | |
| MOTA | | | VAL | 95 | 33.506 | 33.493 | 36.281 | 1.00 17.00 | AAAA |
| ATOM | 763 | CA | | | 33.851 | 33.242 | 34.796 | 1.00 25.15 | AAAA |
| MOTA | 764 | CB | VAL | 95 | | | 34.533 | 1.00 27.19 | AAAA |
| MOTA | 765 | CG1 | VAL | 95 | 35.326 | 33.537 | | | AAAA |
| | 766 | | VAL | 95 | 33.551 | 31.791 | 34.443 | 1.00 17.37 | |
| MOTA | | | | 95 | 33.989 | 34.899 | 36.686 | 1.00 17.42 | AAAA |
| ATOM | 767 | С | VAL | | | 35.894 | 36.237 | 1.00 23.43 | AAAA |
| MOTA | 768 | . O | VAL | 95 | 33.426 | | 37.563 | 1.00 18.84 | AAAA |
| ATOM | 769 | N | SER | 96 | 34.986 | 34.982 | | | AAAA |
| | | CA | SER | 96 | 35.564 | 36.270 | 37.982 | 1.00 21.77 | |
| MOTA | 770 | | | | 34.608 | 37.070 | 38.867 | 1.00 23.11 | AAAA |
| MOTA | 771 | CB | SER | 96 | | | 40.223 | 1.00 24.43 | AAAA |
| MOTA | 772 | OG | SER | 96 | 34.723 | 36.679 | | | AAAA |
| | 773 | С | SER | 96 | 36.835 | 35.987 | 38.789 | 1.00 29.09 | |
| ATOM | | | | 96 | 37.117 | 34.828 | 39.115 | 1.00 27.12 | AAAA |
| ATCM | 774 | 0 | SER | | | 37.020 | 39.124 | 1.00 17.51 | AAAA |
| ATOM | 775 | N | TYR | 97 | 37.610 | | | 1.00 20.69 | AAAA |
| ATOM | 776 | CA | TYR | 97 | 38.803 | 36.751 | 39.911 | 1.00 20.03 | AAAA |
| | | | TYR | 97 | 39.865 | 37.835 | 39.712 | 1.00 21.82 | |
| MOTA | 777 | CB | | | 40.492 | 37.748 | | 1.00 22.72 | AAAA |
| ATOM | 778 | CG | TYR | 97 | | | | | AAAA |
| MOTA | 779 | CD1 | TYR | 97 | 39.936 | 38.414 | | | AAAA |
| | 780 | | TYR | 97 | 40.473 | 38.265 | 35.949 | 1.00 24.45 | |
| ATOM | | | | | 41.599 | | | 1.00 19.74 | AAAA |
| MOTA | 781 | | TYR | 97 | | | | | AAAA |
| ATOM | 782 | CE2 | TYR | 97 | 42.144 | | | | AAAA |
| | 783 | | TYR | 97 | 41.578 | 37.439 | | | |
| MOTA | | | | 97 | 42.122 | | | 1.00 28.54 | AAAA |
| ATOM | 784 | | TYR | | | _ | | | AAAA |
| MOTA | 785 | С | TYR | 97 | 38.510 | | | | AAAA |
| | 786 | | TYR | 97 | 39.413 | 36.285 | | 1.00 19.70 | |
| ATOM | | | | 98 | 37.243 | | 41.764 | 1.00 18.56 | AAAA |
| ATOM | 787 | | ALA | | | | | | AAAA |
| ATOM | 788 | CA | $\lambda L \lambda$ | 98 | 36.899 | | | | AAAA |
| ATOM | 789 | | ALA | 98 | 35.561 | 36.888 | | | AAAA |
| | | | ALA | 98 | 36.776 | 34.743 | 43.224 | | |
| ATOM | 790 | | | | 36.931 | | 44.289 | 1.00 20.14 | AAAA |
| ATOM | 791 | . 0 | ALA | 98 | | 24 004 | | | AAAA |
| | 702 | NT I | MET | 99 | 36.538 | 34.094 | , TE.VO | 1.00 -0.3- | |

| | | | | | 25.225 | 20 642 | 42 317 | 1.00 17.60 | AAAA |
|------|-----|-----|-----|-----|--------|----------|--------|------------|------|
| ATOM | 793 | CA | MET | 99 | 36.295 | 32.643 | 42.117 | 1.00 17.05 | AAAA |
| MOTA | 794 | CB | MĘT | 99 | 35.864 | 32.137 | 40.736 | | AAAA |
| ATOM | 795 | | MET | 99 | 36.999 | 31.824 | 39.793 | 1.00 11.16 | |
| ATOM | 796 | - | MET | 99 | 36.314 | 31.698 | 38.113 | 1.00 16.54 | AAAA |
| | 797 | CE | MET | 99 | 35.165 | 30.295 | 38.312 | 1.00 17.83 | AAAA |
| ATOM | | | MET | 99 | 37.432 | 31.800 | 42.650 | 1.00 18.98 | AAAA |
| ATOM | 798 | C | | 99 | 37.197 | 30.753 | 43.251 | 1.00 18.21 | AAAA |
| MOTA | 799 | 0 | MET | | 38.670 | 32.216 | 42.420 | 1.00 12.87 | AAAA |
| MOTA | 800 | N | PHE | 100 | | 31.439 | 42.987 | 1.00 17.13 | AAAA |
| MOTA | 801 | CA | PHE | 100 | 39.774 | | 41.917 | 1.00 15.23 | AAAA |
| ATOM | 802 | CB | PHE | 100 | 40.559 | 30.681 | | 1.00 15.20 | AAAA |
| ATOM | 803 | CG | PHE | 100 | 41.647 | 29.834 | 42.492 | | AAAA |
| ATOM | 804 | CD1 | PHE | 100 | 41.342 | 28.638 | 43.140 | 1.00 22.96 | |
| ATOM | 805 | CD2 | | 100 | 42.972 | 30.282 | 42.488 | 1.00 17.12 | AAAA |
| | 806 | CE1 | | 100 | 42.341 | 27.901 | 43.782 | 1.00 19.23 | AAAA |
| ATOM | 807 | CE2 | PHE | 100 | 43.974 | 29.552 | 43.129 | 1.00 16.99 | AAAA |
| MOTA | | | PHE | 100 | 43.658 | | 43.779 | 1.00 17.78 | AAAA |
| ATOM | 808 | CZ | | 100 | 40.755 | | 43.774 | 1.00 20.54 | AAAA |
| ATOM | 809 | С | PHE | | 41.088 | | 44.912 | 1.00 21.45 | AAAA |
| ATOM | 810 | 0 | PHE | 100 | 41.219 | | 43.187 | 1.00 18.02 | AAAA |
| MOTA | 811 | N | THR | 101 | | | 43.902 | 1.00 15.25 | AAAA |
| ATOM | 812 | CA | THR | 101 | 42.177 | | 42.976 | 1.00 16.33 | AAAA |
| ATOM | 813 | CB | THR | 101 | 42.715 | | | 1.00 16.01 | AAAA |
| MOTA | 814 | OG1 | THR | 101 | 43.386 | | 41.870 | | AAAA |
| ATOM | 815 | CG2 | THR | 101 | 43.706 | | 43.697 | 1.00 16.31 | AAAA |
| MOTA | 816 | С | THR | 101 | 41.567 | | 45.160 | 1.00 14.12 | |
| | 817 | ō | THR | 101 | 42.110 | 34.707 | 46.244 | 1.00 16.86 | AAAA |
| MOTA | 818 | N | GLY | 102 | 40.435 | 35.541 | 45.008 | 1.00 13.77 | AAAA |
| MOTA | | CA | GLY | 102 | 39.770 | 36.145 | 46.156 | 1.00 16.29 | AAAA |
| MOTA | 819 | | GLY | 102 | 39.330 | | 47.133 | 1.00 16.75 | AAAA |
| MOTA | 820 | С | | 102 | 39.502 | | 48.338 | 1.00 14.48 | AÁAA |
| ATOM | 821 | 0 | GLY | 102 | 38.752 | | 46.615 | 1.00 16.24 | AAAA |
| MOTA | 822 | N | SER | | 38.315 | | 47.488 | 1.00 16.72 | AAAA |
| MOTA | 823 | CA | SER | 103 | | | 46.684 | 1.00 15.97 | AAAA |
| ATOM | 824 | CB | SER | 103 | 37.567 | | 46.197 | 1.00 26.86 | AAAA |
| ATOM | 825 | OG | SER | 103 | 36.339 | | | 1.00 17.88 | AAAA |
| ATOM | 826 | С | SER | 103 | 39.494 | | 48.218 | 1.00 17.33 | AAAA |
| ATOM | 827 | 0 | SER | 103 | 39.405 | | 49.419 | | AAAA |
| ATOM | 828 | N | SER | 104 | 40.604 | | 47.515 | 1.00 11.40 | AAAA |
| MOTA | 829 | CA | SER | 104 | 41.780 | | 48.181 | 1.00 17.61 | AAAA |
| ATOM | 830 | CB | SER | 104 | 42.888 | | 47.160 | 1.00 15.89 | |
| | 831 | OG | SER | 104 | 42.52 | 30.102 | 46.362 | 1.00 27.82 | AAAA |
| ATOM | 832 | C | SER | 104 | 42.332 | 2 32.404 | 49.271 | 1.00 17.02 | AAAA |
| ATOM | | Ö | SER | 104 | 42.86 | | 50.286 | 1.00 15.37 | AAAA |
| ATOM | 833 | | LEU | 105 | 42.20 | | 49.052 | 1.00 17.10 | AAAA |
| ATOM | 834 | N | | 105 | 42.70 | | 50.016 | 1.00 16.95 | AAAA |
| MOTA | 835 | CA | LEU | 105 | 42.72 | | 49.365 | 1.00 18.44 | AAAA |
| ATOM | 836 | CB | LEU | | 43.61 | _ | | 1.00 29.88 | AAAA |
| MOTA | 837 | CG | LEU | 105 | | | 49.959 | 1.00 20.25 | AAAA |
| ATOM | 838 | CD1 | LEU | 105 | 45.08 | | | 1.00 29.39 | AAAA |
| ATOM | 839 | CD2 | LEU | 105 | 43.43 | | | 1.00 14.81 | AAAA |
| ATOM | 840 | С | LEU | 105 | 41.83 | | | 1.00 17.74 | AAAA |
| MOTA | 841 | 0 | LEU | 105 | 42.33 | | | 1.00 17.74 | AAAA |
| ATOM | 842 | N | ALA | 106 | 40.53 | | | | AAAA |
| ATOM | 843 | CA | ALA | 106 | 39.60 | 1 34.493 | | 1.00 12.39 | AAAA |
| ATOM | 844 | CB | ALA | 106 | 38.14 | | | 1.00 11.58 | |
| | 845 | c | ALA | 106 | 39.80 | 7 33.210 | 53.023 | 1.00 14.79 | AAAA |
| MOTA | 846 | ō | ALA | 106 | 39.70 | | 54.250 | 1.00 13.58 | AAAA |
| MOTA | | | THR | 107 | 40.11 | | | 1.00 13.67 | AAAA |
| MOTA | 847 | N | | 107 | 40.31 | | | | AAAA |
| ATOM | 848 | CA | THR | | 40.18 | | _ | | AAAA |
| MOTA | 849 | CB | THR | 107 | 38.86 | | | | AAAA |
| MOTA | 850 | OG | | 107 | 30.00 | | | | AAAA |
| ATOM | 851 | CG2 | | 107 | 40.42 | | | | AAAA |
| ATCM | 852 | С | THR | 107 | 41.64 | | | | AAAA |
| ATCM | 853 | 0 | THR | 107 | 41.73 | | | | AAAA |
| ATOM | 854 | | GLY | 108 | 42.69 | | | | AAAA |
| ATOM | 855 | | GLY | 108 | 43.96 | | | | AAAA |
| ATOM | 856 | | GLY | 108 | 43.80 | 1 32.119 | | | |
| | 857 | | GLY | 108 | 44.41 | | | 1.00 17 53 | AAAA |
| ATOM | 858 | | SER | 109 | 42.96 | | | 1.00 15.26 | AAAA |
| ATCM | 350 | •• | | | | | - | | • |
| | | | | | | | | | |

32/263 Figure 16-14

| ATOM | 859 | CA | SER | 109 | 42,727 | 34.020 | 56.153 | 1.00 14.54 | AAAA |
|--------|-------|-----|--------|-----|--------|----------|--------|------------|-------------|
| | | | | 109 | 41.906 | 35.248 | 55.737 | 1.00 15.58 | AAAA |
| ATOM | 860 | CB | SER | | | - | 54.809 | 1.00 16.97 | AAAA |
| MOTA | 861 | OG | SER | 109 | 42.627 | 36.045 | | | |
| ATOM | 862 | С | SER | 109 | 42.037 | 33.264 | 57.297 | 1.00 15.56 | AAAA |
| ATOM | 863 | 0 | SER | 109 | 42.189 | 33.600 | 58.487 | 1.00 17.00 | AAAA |
| | | | | 110 | 41.261 | 32.247 | 56.944 | 1.00 14.37 | AAAA |
| MOTA | 864 | N | THR | | | | 57.957 | 1.00 12.89 | AAAA |
| ATOM | 865 | CA | THR | 110 | 40.608 | 31.435 | | | |
| ATOM | 866 | CB | THR | 110 | 39.452 | 30.628 | 57.360 | 1.00 14.54 | AAAA |
| | 867 | OG1 | THR | 110 | 38.346 | 31.519 | 57.163 | 1.00 18.11 | AAAA |
| MOTA | | | | 110 | 39.061 | 29.452 | 58.278 | 1.00 12.91 | AAAA |
| MOTA | 868 | CG2 | THR | | | | 58.601 | 1.00 18.44 | AAAA |
| MOTA | 869 | С | THR | 110 | 41.633 | 30.524 | | | |
| ATOM | 870 | 0 | THR | 110 | 41.574 | 30.302 | 59.806 | 1.00 16.30 | AAAA |
| ATOM | 871 | N | VAL | 111 | 42.584 | 30.013 | 57.816 | 1.00 15.20 | AAAA |
| | | CA | VAL | 111 | 43.614 | 29.180 | 58.403 | 1.00 20.45 | AAAA |
| MOTA | 872 | | | | 44.517 | 28.514 | 57.323 | 1.00 20.02 | AAAA |
| MOTA | 873 | CB | VAL | 111 | | | | | |
| ATOM | 874 | CG1 | VAL | 111 | 45.652 | 27.765 | 58.005 | 1.00 21.79 | AAAA |
| ATOM | 875 | CG2 | VAL | 111 | 43.697 | 27.537 | 56.482 | 1.00 19.07 | AAAA |
| | | C | VAL | 111 | 44.456 | 30.075 | 59.327 | 1.00 18.21 | AAAA |
| MOTA | 876 | | | | 44.838 | 29.672 | 60.431 | 1,00 18.65 | AAAA |
| ATOM | 877 | 0 | VAL | 111 | | | | | AAAA |
| MOTA | 878 | N | GLN | 112 | 44.731 | 31.302 | 58.890 | 1.00 16.82 | |
| ATOM | 879 | CA | GLN | 112 | 45.493 | 32.232 | 59.719 | 1.00 20.13 | AAAA |
| | 880 | CB | GLN | 112 | 45.751 | 33.540 | 58.970 | 1.00 22.39 | AAAA |
| MOTA | | | | | 46.593 | 33.360 | 57.723 | 1.00 21.17 | AAAA |
| MOTA | 881 | CG | GLN | 112 | | | | 1.00 24.82 | AAAA |
| MOTA | 882 | CD | GLN | 112 | 46.797 | 34.651 | 56.982 | | |
| MOTA | 883 | OE1 | GLN | 112 | 47.772 | 35.381 | 57.219 | 1.00 25.62 | AAAA |
| ATOM | 884 | NE2 | | 112 | 45.866 | . 34.963 | 56.091 | 1.00 13.16 | አጸጸአ |
| | | | GLN | 112 | 44.743 | 32.516 | 61.012 | 1.00 23.99 | AAAA |
| MOTA | 885 | C | | | | 32.593 | 62.079 | 1.00 17.94 | AAAA |
| MOTA | 886 | 0 | GLN | 112 | 45.340 | | | | AAAA |
| MOTA | 887 | N | ALA | 113 | 43.431 | 32.700 | 60.924 | 1.00 15.60 | |
| ATOM | -888 | CA | ALA | 113 | 42.653 | 32.941 | 62.138 | 1.00 15.04 | AAAA |
| | 889 | СВ | ALA | 113 | 41.191 | 33.138 | 61.802 | 1.00 18.65 | AAAA |
| MOTA | | | | | 42.807 | 31.751 | 63.083 | 1.00 14.84 | AAAA |
| MOTA | 890 | С | ALA | 113 | | | | 1.00 21.05 | AAAA |
| ATOM | 891 | Ο. | ALA | 113 | 42.941 | 31.909 | 64.296 | | |
| ATOM | 892 | N | ILE | 114 | 42.767 | 30.550 | 62.534 | 1.00 16.45 | AAAA |
| MOTA | 893 | CA | ILE | 114 | 42.919 | 29.383 | 63.389 | 1.00 15.38 | AAAA |
| | | | ILE | 114 | 42.600 | 28.100 | 62.637 | 1.00 15.22 | AAAA |
| ATOM | 894 | CB | | | | 26.893 | 63.537 | 1.00 15.72 | AAAA |
| ATOM | 895 | | ILE | 114 | 42.888 | | | | AAAA |
| ATOM | 896 | CG1 | ILE | 114 | 41.110 | 28.112 | 62.244 | 1.00 19.28 | |
| ATOM | 897 | CD1 | ILE | 114 | 40.744 | 27.038 | 61.191 | 1.00 13.43 | AAAA |
| | 898 | c | ILE | 114 | 44.329 | 29.318 | 63.968 | 1.00 18.02 | AAAA |
| ATOM | • | | | 114 | 44.508 | 28.998 | 65.156 | 1.00 20.38 | AAAA |
| MOTA | 899 | 0 | ILE | | | | 63.144 | 1.00 15.27 | AAAA |
| MOTA | 900 | N | GLU | 115 | 45.328 | 29.629 | | | |
| MOTA | 901 | CA | GLU | 115 | 46.726 | 29.626 | 63.614 | 1.00 21.48 | AAAA |
| ATOM | 902 | CB | GLU | 115 | 47.690 | 30.080 | 62.506 | 1.00 21.76 | AAAA |
| | 903 | CG | GLU | 115 | 47.884 | 29.080 | 61.386 | 1.00 15.78 | AAAA |
| MOTA | - | | | | | 29.648 | 60.211 | 1.00 20.04 | AAAA |
| MO £ | 904 | CD | GLU | 115 | 48.670 | | | | AAAA |
| A COM | 905 | 0E1 | GLU | 115 | 49.051 | 30.843 | 60.239 | 1.00 21.48 | |
| A.OM | 906 | OE2 | GLU | 115 | 48.901 | 28.902 | 59.241 | 1.00 26.59 | AAAA |
| | 907 | C | GLU | 115 | 46.877 | 30.559 | 64.814 | 1.00 23.55 | AAAA |
| MOTA | | | | | 47.509 | 30.212 | 65.815 | 1.00 23.03 | AAAA |
| ATOM | 908 | 0 | GLU | 115 | | | | 1.00 22.73 | AAAA |
| ATOM | 909 | N | GLU | 116 | 46.295 | 31.748 | 64.703 | | |
| MOTA | 910 | CA | GLU | 116 | 46.367 | 32.735 | 65.774 | 1.00 20.54 | AAAA |
| ATOM | 911 | CB | GLU | 116 | 45.744 | 34.044 | 65.320 | 1.00 18.40 | AAAA |
| | | ĊĠ | GLU | 116 | 46.562 | 34.765 | 64.279 | 1.00 19.76 | AAAA |
| MOTA | . 912 | | | | | 34.998 | 64.756 | 1.00 27.24 | AAAA |
| MOTA | 913 | CD | GLU | 116 | 47.985 | | | | AAAA |
| MOTA | 914 | | GLU | 116 | 48.164 | 35.630 | 65.815 | 1.00 18.44 | |
| MOTA | 915 | CE2 | GLU | 116 | 48.919 | | 64.078 | 1.00 23.17 | AAAA |
| | 916 | c | GLU | 116 | 45.682 | 32.253 | 67.034 | 1.00 25.39 | AAAA |
| MOTA | | | | | | 32.427 | 68.137 | 1.00 22.87 | AAAA |
| MOTA | 917 | 0 | GLU | 116 | 46.207 | | | | AAAA |
| ATOM | 918 | И | PHE | 117 | 44.510 | 31.647 | 66.872 | 1.00 18.78 | |
| ATOM | 919 | CA | PHE | 117 | 43.778 | 31.139 | 68.019 | 1.00 22.11 | AAAA |
| | 920 | CB | PHE | 117 | 42.451 | 30.530 | 67.581 | 1.00 23.14 | AAAA |
| MOTA | | | | | | 30.054 | 68.728 | 1.00 24.06 | AAAA |
| ATOM | 921 | CG | PHE | 117 | 41.603 | | | 1.00 19.67 | AAAA |
| ATOM | 922 | CD1 | PHE | 117 | 40.880 | 30.961 | 69.493 | | |
| . ATOM | 923 | CD2 | PHE | 117 | 41.559 | 28.701 | 69.066 | 1.00 24.08 | AAAA |
| | 924 | | PHE | 117 | 40.115 | 30.531 | 70.586 | 1.00 23.68 | AAAA |
| ATOM | 764 | | E. LIE | | | | | | |

| | | _ | | | 40.799 | 28.262 | 70.156 | 1.00 24.04 | AAAA |
|--------|-----|-----------|-------|-----|--------|---------|----------|------------|------|
| MOTA | | CE2 | | 117 | | 29.179 | 70.915 | 1.00 19.62 | AAAA |
| MOTA | 926 | CZ | PHE | 117 | 40.078 | | 68.747 | 1.00 23.87 | AAAA |
| ATOM | 927 | С | PHE | 117 | 44.587 | 30.068 | | 1.00 24.40 | AAAA |
| MOTA | | 0 | PHE | 117 | 44.613 | 30.031 | 69.979 | 1.00 21.09 | AAAA |
| ATOM | | N | LEU. | 118 | 45.238 | 29.194 | 67.981 | | AAAA |
| | | | LEU | 118 | 46.025 | 28:113 | 68.549 | 1.00 20.73 | |
| ATOM | • | | LEU | 118 | 46.358 | 27.075 | 67.480 | 1.00 17.90 | AAAA |
| MOTA | | | LEU | 118 | 45.148 | 26.264 | 66.984 | 1.00 26.20 | AAAA |
| MOTA | | CG CD1 | | 118 | 45.591 | 25.288 | 65.924 | 1.00 34.23 | AAAA |
| MOTA | | | | 118 | 44.520 | 25.499 | 68.139 | 1.00 27.16 | AAAA |
| MOTA | | CD2 | | | 47.290 | 28.601 | 69.238 | 1.00 26.49 | AAAA |
| MOTA | | | LEU | 118 | 47.908 | 27.856 | 69.996 | 1.00 26.34 | AAAA |
| ATOM | 936 | | LEU | 118 | 47.672 | 29.848 | 68.975 | 1.00 28.92 | AAAA |
| MOTA | 937 | | LYS | 119 | | 30.459 | 69.624 | 1.00 28.53 | AAAA |
| ATOM | 938 | | LYS | 119 | 48.835 | | 68.805 | 1.00 30.15 | AAAA |
| ATOM | 939 | CB | LYS | 119 | 49.392 | 31.616 | 67.437- | 1.00 35.14 | AAAA |
| ATOM | 940 | CG | LYS | 119 | 49.915 | 31.267 | 66.716 | 1.00 28.98 | AAAA |
| ATOM | 941 | CD | LYS | 119 | 50.291 | 32.549 | | 1.00 31.07 | AAAA |
| ATOM | 942 | CE | LYS | 119 | 50.905 | 32.262 | 65.380 | 1.00 31.07 | AAAA |
| ATOM | 943 | NZ | LYS | 119 | 51.195 | 33.551 | 64.745 | | AAAA |
| | 944 | C | LYS | 119 | 48.335 | 31.053 | 70.932 | 1.00 35.74 | AAAA |
| MOTA | 945 | 0 | LYS | 119 | 49.117 | 31.541 | 71.750 | 1.00 27.10 | AAAA |
| MOTA | | N | GLY | 120 | 47.018 | 31.050 | 71.103 | 1.00 25.20 | |
| MOTA | 946 | | GLY | 120 | 46.445 | 31.605 | 72.309 | 1.00 30.18 | AAAA |
| MOTA | 947 | CA | | 120 | 45.913 | 33.007 | 72.122 | 1.00 31.91 | AAAA |
| MOTA | 948 | C | GLY | 120 | 45.540 | 33.665 | 73.094 | 1.00 34.76 | AAAA |
| MOTA | 949 | 0 | GLY | 121 | 45.889 | 33.495 | 70.887 | 1.00 20.56 | AAAA |
| MOTA | 950 | N | ASN | | 45.353 | 34.825 | 70.681 | 1.00 25.58 | AAAA |
| MOTA | 951 | CA | ASN | 121 | 46.278 | 35.634 | 69.785 | 1.00 29.99 | AAAA |
| MOTA | 952 | CB | ASN | 121 | | 35.827 | 70.427 | 1.00 24.43 | AAAA |
| MOTA | 953 | CG | ASN | 121 | 47.641 | 34.874 | 70.588 | 1.00 54.63 | AAAA |
| MOTA | 954 | | ASN | 121 | 48.396 | 37.045 | 70.817 | 1.00 41.69 | AAAA |
| ATOM | 955 | ND2 | ASN | 121 | 47.944 | | 70.135 | 1.00 18.85 | AAAA |
| ATOM | 956 | С | ASN | 121 | 43.941 | 34.759 | 69.899 | 1.00 24.77 | AAAA |
| MOTA | 957 | 0 | ASN | 121 | 43.421 | | 69.991 | 1.00 19.55 | AAAA |
| ATOM | 958 | N. | VAL | 122 | 43.310 | | | 1.00 22.90 | AAAA |
| ATOM | 959 | CA | VAL | 122 | 41.936 | | 69.499 | 1.00 22.30 | AAAA |
| ATOM | 960 | CB | VAL | 122 | 41.053 | | 70.449 | | AAAA |
| | 961 | | VAL | 122 | 39.649 | | 69.851 | 1.00 31.52 | AAAA |
| MOTA | 962 | | VAL | 122 | 40.986 | 36.154 | 71.810 | 1.00 32.50 | AAAA |
| ATOM . | 963 | C | VAL | 122 | 41.953 | 36.632 | 68.130 | 1.00 16.87 | AAAA |
| ATOM | 964 | 0 | VAL | 122 | 42.518 | 37.710 | 67.938 | 1.00 24.08 | AAAA |
| MOTA | 965 | N | ALA | 123 | 41.321 | 35.983 | 67.159 | 1.00 18.67 | AAAA |
| MOTA | | | ALA | 123 | 41.360 | 36.532 | 65.821 | 1.00 10.18 | |
| MOTA | 966 | CA | ALA | 123 | 42.346 | | 64.990 | 1.00 19.04 | AAAA |
| MOTA | 967 | CB | | 123 | 40.000 | | 65.131 | 1.00 13.72 | AAAA |
| MOTA | 968 | C | ALA | 123 | 39.108 | | | 1.00 20.78 | AAAA |
| ATOM | 969 | 0 | ALA | 123 | 39.871 | | | 1.00 12.92 | AAAA |
| ATOM | 970 | N | PHE | _ | 38.649 | | | 1.00 14.67 | AAAA |
| ATOM | 971 | CA | PHE | 124 | 37.904 | 38.878 | | 1.00 14.67 | AAAA |
| ATCM | 972 | CB | PHE | 124 | 36.660 | 39.209 | | | AAAA |
| MOTA | 973 | CG | PHE | 124 | | | | | AAAA |
| ATOM | 974 | | PHE | 124 | 35.81 | | | | AAAA |
| ATOM | 975 | | PHE | 124 | 36.286 | | | | AAAA |
| ATOM | 976 | CEI | PHE | 124 | 34.609 | | | | AAAA |
| MOTA | 977 | CE2 | PHE | 124 | 35.072 | | | | AAAA |
| ATOM | 978 | CZ | PHE | 124 | 34.24 | | | | AAAA |
| | 979 | Ċ | PHE | 124 | 39.01 | | | | AAAA |
| ATOM | 980 | ō | PHE | 124 | 39.82 | 38.558 | 61.535 | | AAAA |
| MOTA | | | ASN | 125 | 38.44 | | 61.126 | 1.00 19.39 | AAAA |
| ATOM | 981 | И | ASN | 125 | 38.65 | | 59.691 | | |
| ATOM | 982 | CA | | 125 | 39.12 | | 7 59.150 | | AAAA |
| MOTA | 983 | CB | ASN | 125 | 39.06 | | | 1.00 12.84 | AAAA |
| ATCM | 984 | CG | ASN | | 39.21 | | | 1.00 14.91 | AAAA |
| MOTA | 985 | | 1 ASN | 125 | 38.85 | | | 1.00 16.21 | AAAA |
| ATOM | 986 | ND: | 2 ASN | 125 | 37.31 | | | | AAAA |
| ATCM | 987 | С | ASN | 125 | | | | | AAAA |
| ATOM | 988 | 0 | ASN | 125 | 36.50 | | | | AAAA |
| ATOM | 989 | N | PRO | 126 | 37.07 | | | | AAAA |
| ATCM | 990 | | PRO | 126 | 37.90 | 8 39.68 | 29.00 | | • |
| | | | | | | | | | |
| | | | | | | | | | |

| | 991 | CA PI | RO | 126 | | 35.811 | 38.910 | 58.156 | 1.00 17.33 | AAAA |
|--------|------|-------|-----|-----|---|--------|--------|----------|------------|-------|
| ATOM | | | RO | 126 | | 35.912 | 40.434 | 58.177 | 1.00 16.32 | AAAA |
| MOTA | 992 | | | 126 | | 37.416 | 40.655 | 58.008 | 1.00 20.95 | AAAA |
| MOTA | 993 | | RO | | | 35.549 | 38.359 | 56.752 | 1.00 13.78 | AAAA |
| MOTA | 994 | C P | RO | 126 | | | | 56.322 | 1.00 17.03 | AAAA |
| ATOM | 995 | 0 P | RO | 126 | | 34.404 | 38.291 | | | AAAA |
| ATOM - | 996 | N A | LA | 127 | | 36.607 | 37.972 | 56.042 | 1.00 14.57 | |
| | 997 | | LA | 127 | • | 36.463 | 37.443 | 54.691 | 1.00 17.37 | AAAA |
| MOTA | | | | 127 | | 37.816 | 37.540 | 53.930 | 1.00 14.48 | AAAA |
| MOTA | 998 | | LA | | | 35.982 | 35.998 | 54.702 | 1.00 19.77 | AAAA |
| ATOM | 999 | _ | LA | 127 | | | | 53.688 | 1.00 15.62 | AAAA |
| ATOM | 1000 | O A | LA | 127 | | 35.490 | 35.500 | | 1.00 13.54 | AAAA |
| | 1001 | | LY | 128 | | 36.111 | 35.339 | 55.849 | | |
| MOTA | | | LY | 128 | | 35.725 | 33.939 | 55.971 | 1.00 13.53 | AAAA |
| MOTA | 1002 | | | 128 | • | 34.234 | 33.679 | 56.101 | 1.00 14.49 | AAAA |
| MOTA | 1003 | - | LY | | | 33.414 | 34.585 | 56.017 | 1.00 15.65 | AAAA |
| MOTA | 1004 | | LY | 128 | | | | 56.314 | 1.00 13.35 | AAAA |
| ATOM | 1005 | N G | LY | 129 | | 33.883 | 32.420 | | 1.00 16.28 | -AAAA |
| ATOM | 1006 | CA G | LY | 129 | | 32.487 | 32.058 | 56.446 | | AAAA |
| | 1007 | | LY | 129 | | 31.754 | 31.831 | 55.130 | 1.00 15.69 | |
| MOTA | | _ | LY | 129 | | 30.543 | 32.021 | 55.072 | 1.00 16.10 | AAAA |
| ATOM | 1008 | | | | | 32.479 | 31.448 | 54.079 | 1.00 15.00 | AAAA |
| MOTA | 1009 | - | ŒΤ | 130 | | | | 52.757 | 1.00 13.35 | AAAA |
| MOTA | 1010 | CA M | 1ET | 130 | | 31.879 | 31.163 | | 1.00 12.20 | AAAA |
| ATOM | 1011 | CB M | 1ET | 130 | | 32.969 | 31.215 | 51.689 | | AAAA |
| | 1012 | | 1ET | 130 | | 33.680 | 32.573 | 51.731 | 1.00 17.03 | |
| ATOM | | | 1ET | 130 | | 34.863 | 32.877 | 50.425 | 1.00 15.41 | AAAA |
| MOTA | 1013 | | | 130 | | 33.752 | 32.973 | 49.073 | 1.00 46.82 | AAAA |
| ATOM | 1014 | | 1ET | | | | 29.756 | 52.885 | 1.00 12.49 | AAAA |
| MOTA | 1015 | C M | 1ET | 130 | | 31.296 | | 52.297 | 1.00 19.54 | AAAA |
| ATOM | 1016 | o M | 1ET | 130 | | 31.785 | 28.789 | | 1.00 16.24 | AAAA |
| ATOM | 1017 | | HIS | 131 | | 30.188 | 29.695 | 53.617 | | |
| | 1018 | - | HIS | 131 | | 29.556 | 28.448 | 54.014 | 1.00 13.80 | AAAA |
| MOTA | | | HIS | 131 | | 28.772 | 28.694 | 55.316 | 1.00 15.91 | AAAA |
| MOTA | 1019 | | | | | 27.606 | 29.625 | 55.175 | 1.00 13.08 | AAAA |
| ATOM | 1020 | | HIS | 131 | | | | 56.096 | 1.00 12.46 | AAAA |
| ATOM | 1021 | CD2 I | HIS | 131 | | 26.712 | 30.063 | | 1.00 22.48 | AAAA |
| ATOM | 1022 | ND1 F | HIS | 131 | | 27.225 | 30.190 | 53.976 | | AAAA |
| | 1023 | CE1 F | | 131 | | 26.148 | 30.936 | 54.166 | 1.00 16.56 | |
| ATOM | | NE2 | | 131 | | 25.817 | 30.875 | 55.442 | 1.00 23.56 | AAAA |
| MOTA | 1024 | | | 131 | | 28.673 | 27.663 | 53.066 | 1.00 13.69 | AAAA |
| MOTA | 1025 | | HIS | | | 28.125 | 26.658 | 53.470 | 1.00 17.21 | AAAA |
| MOTA | 1026 | | HIS | 131 | | | 28.115 | 51.830 | 1.00 14.51 | AAAA |
| MOTA | 1027 | N I | HIS | 132 | | 28.523 | | | 1.00 20.19 | AAAA |
| ATOM | 1028 | CA I | HIS | 132 | | 27.669 | 27.400 | 50.887 | 1.00 17.26 | AAAA |
| ATOM | 1029 | | HIS | 132 | | 26.863 | 28.416 | 50.054 | 1.00 17.26 | |
| | 1030 | | HIS | 132 | | 25.748 | 29.070 | 50.810 | 1.00 16.85 | AAAA |
| MOTA | | | | 132 | | 24.787 | 28.542 | 51.604 | 1.00 13.74 | AAAA |
| MOTA | 1031 | CD2 | H12 | | | 25.497 | 30.424 | 50.756 | 1.00 24.80 | AAAA |
| MOTA | 1032 | ND1 | | 132 | | | 30.700 | 51.486 | 1.00 12.68 | AAAA |
| MOTA | 1033 | CE1 | HIS | 132 | | 24.429 | | 52.010 | 1.00 28.65 | AAAA |
| ATOM | 1034 | NE2 | HIS | 132 | | 23.980 | 29.576 | | 1.00 16.89 | AAAA |
| ATOM | 1035 | | HIS | 132 | | 28.372 | 26.412 | 49.946 | | AAAA |
| | | | HIS | 132 | | 27.731 | 25.487 | | 1.00 14.58 | |
| ATOM | 1036 | | ALA | 133 | | 29.669 | 26.580 | 49.689 | 1.00 16.79 | AAAA |
| MOTA | 1037 | | | | | 30.338 | 25.680 | 48.740 | 1.00 13.76 | AAAA |
| ATOM | 1038 | | ALA | 133 | | | 26.194 | | 1.00 14.95 | AAAA |
| ATOM | 1039 | CB | ALA | 133 | | 31.738 | | | 1.00 18.80 | AAAA |
| ATOM | 1040 | С | ALA | 133 | | 30.418 | 24.219 | | | AAAA |
| ATOM | 1041 | | ALA | 133 | | 30.557 | 23.939 | | | AAAA |
| | | | PHE | 134 | | 30.306 | 23.306 | 48.209 | 1.00 13.76 | |
| MOTA | 1042 | | | | | 30.378 | 21.868 | 48.451 | 1.00 19.77 | AAAA |
| MOTA | 1043 | | PHE | 134 | | 29.311 | 21.132 | | 1.00 15.59 | AAAA |
| MOTA | 1044 | | PHE | 134 | | | 21.525 | | | AAAA |
| MOTA | 1045 | CG | PHE | 134 | | 27.917 | | | | AAAA |
| MOTA | 1046 | CD1 | PHE | 134 | | 27.135 | 22.259 | | | AAAA |
| | 1047 | CD2 | | 134 | | 27.392 | 21.187 | 49.222 | 1.00 21.68 | |
| MOTA | | | | 134 | | 25.836 | 22.653 | | 1.00 23.07 | AAAA |
| MOTA | 1048 | CE1 | | | | 26.099 | 21.578 | | 1.00 17.64 | AAAA |
| MOTA | 1049 | CE2 | | 134 | | | | | | AAAA |
| ATOM | 1050 | CZ | PHE | 134 | | 25.323 | 22.308 | | | AAAA |
| ATOM | 1051 | C | PHE | 134 | | 31.763 | 21.354 | | | AAAA |
| | 1052 | 5 | PHE | 134 | | 32.547 | 22.049 | | | AAAA |
| MOTA | | | LYS | 135 | | 32.060 | 20.124 | | | |
| MOTA | 1053 | 74 | | 135 | | 33.369 | 19.551 | | 1.00 16.24 | AAAA |
| ATOM | 1054 | ΞÀ | LYS | | | 33.360 | | | 1.00 21.29 | AAAA |
| MOTA | 1055 | | LYS | 135 | | | | | | AAAA |
| MOTA | 1056 | | LYS | 135 | | 34.640 | 17.300 | , 10.400 | | • |
| | | | | | | | | | | |

| | | | | | 1.6-0 | | | | |
|--------------|--------------|-------------|------------|------------|------------------|----------|---------|--------------|--------------|
| | | | | | 24 507 | 15.867 | 48.977 | 1.00 30.26 | AAAA |
| ATOM | 1057 | | LYS | 135 | 34.597 | 15.805 | 50.486 | 1.00 35.01 | AAAA ' |
| MOTA | 1058 | | LYS | 135 | 34.862 | | 50.895 | 1.00 20.61 | AAAA |
| ATOM | 1059 | | LYS | 135 | 36.304 | | 46.836 | 1.00 16.60 | AAAA |
| MOTA | 1060 | | LYS | 135 | 33.854 35.020 | | 46.584 | 1.00 17.24 | AAAA |
| ATOM | 1061 | 0 | LYS | 135 | | | 45.893 | 1.00 18.01 | AAAA |
| ATOM | 1062 | N | SER | 136 | 32.944 | | 44.490 | 1.00 15.26 | AAAA |
| MOTA | 1063 | CA | SER | 136 | 33.301 | 18.094 | 43.940 | 1.00 18.07 | AAAA |
| ATOM | 1064 | CB | SER | 136 | 33.339 | 17.261 | 44.762 | 1.00 22.22 | AAAA |
| ATOM | 1065 | OG | SER | 136 | 34.135 32.345 | 20.355 | 43.658 | 1.00 15.40 | AAAA |
| MOTA | 1066 | С | SER | 136 | 32.162 | 20.071 | 42.475 | 1.00 18.77 | AAAA |
| MOTA | 1067 | 0 | SER | 136 | 31.754 | 21.401 | 44.237 | 1.00 19.71 | · AAAA |
| MOTA | 1068 | И | ARG | 137 | 30.805 | 22.216 | 43.482 | 1.00 17.29 | AAAA . |
| MOTA | 1069 | CA | ARG | 137 | 29.481 | 21.448 | 43.366 | 1.00 24.19 | AAAA |
| MOTA | 1070 | CB | ARG | 137 | | 22.273 | 42.937 | 1.00 32.56 | AAAA |
| MOTA | 1071 | CG | ARG | | 28.290 | 21.424 | 42.980 | 1.00 47.98 | AAAA |
| ATOM | 1072 | CD | ARG | 137 | 26.951 | 20.493 | 41.862 | 1.00 50.95 | AAAA |
| MOTA | 1073 | NE | ARG | 137 | 26.392 | 20.781 | 40.691 | 1.00 50.38 | AAAA |
| MOTA | 1074 | CZ | ARG | 137 | 25.854 | 21.976 | 40.485 | 1.00 45.26 | AAAA |
| MOTA | 1075 | | ARG | 137 | 26.375 | 19.876 | 39.722 | 1.00 55.31 | AAAA |
| MOTA | 1076 | | ARG | 137 | 30.537 | 23.595 | 44.095 | 1.00 16.14 | AAAA |
| MOTA | 1077 | C | ARG | 137 | 30.439 | 23.711 | 45.308 | 1.00 16.88 | AAAA |
| MOTA | 1078 | 0 | ARG | 137 | 30.395 | 24.621 | 43.252 | 1.00 18.07 | AAAA |
| MOTA | 1079 | N | ALA | 138 | 30.117 | 25.976 | 43.735 | 1.00 21.48 | AAAA |
| MOTA | 1080 | CA | ALA | 138 | 30.460 | 27.024 | 42.631 | 1.00 16.55 | AAAA |
| MOTA | 1081 | CB | ALA | 138 | 28.642 | 26.090 | 44.135 | 1.00 21.04 | AAAA |
| ATOM | 1082 | C | ALA | 138 | 27.798 | 25.339 | 43.641 | 1.00 18.97 | AAAA |
| MOTA | 1083 | 0 | ALA | 138 | 28.321 | 27.019 | 45.029 | 1.00 13.83 | AAAA |
| MOTA | 1084 | N | ASN | 139 | 26.952 | 27.158 | 45.468 | 1.00 12.92 | AAAA |
| MOTA | 1085 | CA | ASN | 139 139 | 26.566 | 25.899 | 46.274 | 1.00 13.14 | AAAA |
| ATOM | 1086 | CB | ASN | | 25.162 | 25.961 | 46.832 | 1.00 20.34 | AAAA |
| MOTA | 1087 | CG | ASN | 139 | 24.186 | 26.068 | 46.086 | 1.00 19.76 | AAAA |
| MOTA | 1088 | | ASN | 139 139 | 25.048 | 25.881 | | 1.00 16.36 | AAAA |
| MOTA | 1089 | | ASN | 139 | 26.756 | 28.409 | 46.315 | 1.00 20.92 | AAAA |
| MOTA | 1090 | C | ASN | 139 | 27.603 | 28.738 | 47.148 | 1.00 16.81 | AAAA |
| ATOM | 1091 | 0 | ASN | 140 | 25.644 | 29.105 | 46.086 | 1.00 19.30 | AAAA |
| MOTA | 1092 | N | GLY | 140 | 25.330 | 30.295 | 46.864 | 1.00 21.34 | AAAA |
| MOTA | 1093 | CA | GLY GLY | 140 | 26.393 | | 46.888 | 1.00 20.19 | AAAA |
| MOTA | 1094 | C | GLY | 140 | 26.653 | 31.968 | 47.943 | 1.00 18.77 | AAAA AAAA |
| MOTA | 1095 | 0 | PHE | 141 | 26.996 | 31.649 | 45.733 | 1.00 15.52 | AAAA |
| MOTA | 1096 | N | PHE | 141 | 28.034 | | 45.600 | 1.00 20.71 | AAAA |
| MOTA | 1097 | CA | PHE | 141 | 27.711 | | 46.388 | 1.00 20.03 | AAAA |
| ATOM | 1098 | CB CG | PHE | 141 | 26.355 | | 46.127 | 1.00 28.32 | AAAA |
| MOTA | 1099 | | 1 PHE | 141 | 25.855 | 35.526 | 46.997 | | AAAA |
| MOTA | 1100 1101 | | 2 PHE | 141 | 05 500 | 34.170 | 45.029 | | AAAA |
| MOTA | 1101 | CE. | 1 PHE | 141 | 24.628 | 36.116 | 46.775 | 1.00 25.94 | AAAA |
| ATOM | 1102 | | 2 PHE | 141 | 24.346 | 34.766 | 44.801 | | AAAA |
| MOTA | 1103 | | | 141 | 23.870 | | | | AAAA |
| MOTA | 1105 | | PHE | 141 | 29.357 | | | | AAAA |
| MOTA | 1105 | | PHE | 141 | 30.336 | 32.914 | | | AAAA |
| MOTA | 1107 | | CYS | 142 | 29.389 | | | | AAAA |
| MOTA MOTA | 1108 | | | 142 | 30.629 | 30.466 | | | AAAA |
| | 1109 | | | 142 | 30.347 | 29.845 | | | AAAA |
| MOTA MOTA | 1110 | | | 142 | 29.606 | | | | AAAA |
| | 1111 | | CYS | 142 | 31.313 | | | 44 60 | AAAA |
| MOTA | 1112 | | CYS | 142 | 30.64 | 7 28.527 | | | AAAA |
| MOTA | 1113 | | TYR | 143 | 32.639 | 29.539 | | | AAAA |
| MOTA MOTA | | | | 143 | 33.42 | | | | AAAA |
| | _ | | _ | 143 | 34.33 | | | | AAAA |
| MOTA | | | | 143 | 33.61 | | 43.61 | | AAAA |
| MOTA | | | 1 TYR | 143 | 33.39 | | | 00 | AAAA |
| ATOM | | . כב קרד | 1 TYR | 143 | 32.74 | | | | AAAA |
| MOTA | | | 2 TYR | | 33.15 | 7 29.999 | | | AAAA |
| ATOM | | | | | 32.50 | 1 30.93 | | | AAAA |
| ATOM | | | | | 32.30 | 1 32.22 | | | AAAA |
| ATOM | | - | | | 31.69 | 8 33.17 | 7 41.20 | 0 1.00 10.07 | • |
| ATOM | | _ | | | | | | | |
| | | | | | | | | | |

| | 1123 | С | TYR | 143 | 3 | 4.310 | 27.723 | 46.358 | 1.00 17.35 | | AAAA |
|--------------|--------------|-----|-------|------------|-----|------------------|------------------|------------------|-------------------------|---|--------------|
| ATOM | 1124 | _ | TYR | 143 | 3 | 4.581 | 26.574 | 46.013 | 1.00 16.67 | | AAAA |
| MOTA | 1125 | | ILE | 144 | | 4.763 | 28.262 | 47.489 | 1.00 14.93 | | AAAA |
| ATOM | 1125 | | ILE | 144 | 3 | 5.599 | 27.500 | 48.408 | 1.00 14.17 | | AAAA |
| MOTA | 1127 | | ILE | 144 | 3 | 7.018 | 28.069 | 48.440 | 1.00 14.87 | | AAAA |
| MOTA | 1128 | CG2 | | 144 | 3 | 7.864 | 27.332 | 49.474 | 1.00 13.55 | | AAAA |
| ATOM | 1129 | CG1 | | 144 | 3 | 7.611 | 28.027 | 47.021 | 1.00 16.98 | | AAAA |
| ATOM | 1130 | CD1 | TLE | 144 | 3 | 9.052 | 28.537 | 46.901 | 1.00 17.42 | | AAAA |
| MOTA | 1131 | C | ILE | 144 | 3 | 4.959 | 27.615 | 49.788 | 1.00 17.22 | | AAAA |
| MOTA | 1132 | 0 | ILE | 144 | 3 | 4.606 | 28.716 | 50.220 | 1.00 14.72 | | AAAA |
| ATOM | | N | ASN | 145 | 3 | 4.798 | 26.486 | 50.474 | 1.00 13.46 | | AAAA |
| ATOM | 1133 1134 | CA | ASN | 145 | 3 | 4.170 | 26.493 | 51.797 | 1.00 16.09 | | AAAA |
| ATOM | 1135 | CB | ASN | 145 | | 3.401 | 25.178 | 51.988 | 1.00 14.50 | | AAAA |
| MOTA | 1135 | CG | ASN | 145 | 3 | 2.428 | 25.239 | 53.148 | 1.00 15.64 | | AAAA |
| ATOM | 1137 | OD1 | | 145 | . 3 | 32.800 | 25.587 | 54.263 | 1.00 14.97 | | AAAA |
| MOTA | 1138 | ND2 | | 145 | 3 | 31.170 | 24.916 | 52.882 | 1.00 16.74 | | AAAA |
| ATOM | 1139 | C | ASN | 145 | 3 | 35.266 | 26.639 | 52.873 | 1.00 15.04 | | AAAA AAAA |
| MOTA | 1140 | Ö | ASN | 145 | | 35.812 | 25.637 | 53.338 | 1.00 15.72 | | |
| ATOM | 1141 | N ' | ASN | 146 | 3 | 35.599 | 27.865 | 53.282 | 1.00 12.34 | | AAAA |
| MOTA | 1142 | CA | ASN | 146 | - 1 | 36.685 | 28.006 | 54.262 | 1.00 15.31 | | AAAA AAAA |
| ATOM ATOM | 1143 | CB | ASN | 146 | : | 37.161 | 29.464 | 54.354 | 1.00 15.81 | | AAAA |
| MOTA | 1144 | CG | ASN | 146 | : | 36.101 | 30.396 | 54.865 | 1.00 15.25 | | AAAA |
| ATOM | 1145 | | ASN | 146 | : | 36.113 | 30.757 | 56.034 | 1.00 13.57 | | AAAA |
| ATOM | 1146 | | ASN | 146 | | 35.156 | 30.775 | 53.996 | 1.00 10.85 | | AAAA |
| ATOM | 1147 | C | ASN | 146 | | 36.306 | 27.400 | 55.613 | 1.00 13.04 | | AAAA |
| ATOM | 1148 | ō | ASN | 146 | | 37.160 | 26.865 | 56.314 | 1.00 14.76 | | AAAA |
| ATOM | 1149 | N | PRO | 147 | | 35.025 | 27.489 | 56.016 | 1.00 14.28 | | AAAA |
| ATOM | 1150 | CD | PRO | 147 | | 33.817 | 28.175 | 55.515 | 1.00 7.62 1.00 13.51 | | AAAA |
| MOTA | 1151 | CA | PRO | 147 | | 34.750 | 26.843 | 57.307 | 1.00 13.31 | | AAAA |
| ATOM | 1152 | CB | PRO | 147 | | 33.251 | 27.058 | 57.482 | 1.00 14.44 | | AAAA |
| MOTA | 1153 | CG | PRO | 147 | | 33.056 | 28.436 | 56.827 | 1.00 12.32 | | AAAA |
| MOTA | 1154 | C | PRO | 147 | | 35.118 | 25.330 | 57.278 | 1.00 16.24 | | AAAA |
| ATOM | 1155 | 0 | PRO | 147 | | 35.678 | 24.796 | 58.251 | 1.00 15.24 | | AAAA |
| ATOM | 1156 | N | ALA | 148 | | 34.818 | 24.642 | 56.171 | 1.00 15.58 | | AAAA |
| ATOM | 1157 | CA | ALA | 148 | | 35.122 | 23.200 | 56.080 54.882 | 1.00 13.33 | | AAAA |
| ATOM | 1158 | CB | ALA | 148 | | 34.402 | 22.561 | 55.984 | 1.00 14.94 | | AAAA |
| MOTA | 1159 | С | ALA | 148 | | 36.624 | 22.956 | 56.560 | 1.00 14.69 | | AAAA |
| MOTA | 1160 | 0 | ALA | 148 | | 37.138 | 21.999 23.817 | 55.263 | 1.00 12.49 | | AAAA |
| MOTA | 1161 | N | VAL | 149 | | 37.328 | | 55.163 | 1.00 15.31 | | AAAA |
| MOTA | 1162 | CA | VAL | 149 | | 38.778 | | 54.243 | 1.00 14.77 | | AAAA |
| ATOM | 1163 | CB | VAL | 149 | | 39.364 | | 54.369 | 1.00 14.68 | | AAAA |
| ATOM | 1164 | CG1 | | 149 | | 40.899 | | 52.808 | 1.00 12.50 | | AAAA |
| ATOM | 1165 | CG2 | | 149 | | 38.981 39.323 | | 56.572 | 1.00 20.14 | | AAAA |
| ATOM | 1166 | С | VAL | 149 | | 40.172 | | 57.028 | 1.00 17.32 | | AAAA |
| ATOM | 1167 | 0 | VAL | 149 | | | - 4 | | | | AAAA |
| ATOM | 1168 | N | GLY | 150 | | 38.815 39.284 | | | | | AAAA |
| ATOM | 1169 | CA | GLY | -50 -50 | | 39.030 | | | | | AAAA |
| ATOM | 1170 | C. | GLY | _30 | | 39.888 | | | | | AAAA |
| MOTA | 1171 | 0 | GLY | 150 | | 37.842 | | | 1.00 16.67 | | AAAA |
| ATOM | 1172 | Ŋ | ILE | 151 | | 37.490 | | | 1.00 19.56 | | AAAA |
| MOTA | 1173 | CA | ILE | 151 | | 35.992 | | | 1.00 16.46 | | AAAA |
| ATOM | 1174 | CB | ILE | 151 | | 35.667 | | | 1.00 17.93 | | AAAA |
| ATOM | 1175 | CG2 | | 151 | | 35.180 | | | 1.00 12.31 | | AAAA |
| ATOM | 1176 | CG1 | | 151 | | 33.686 | | | 1.00 18.71 | | AAAA |
| MOTA | 1177 | CD: | | 151 | | 38.352 | | | 1.00 22.66 | | AAAA |
| MOTA | 1178 | Ç | ILE | 151 | | 38.796 | | | 1.00 20.08 | | aaaa |
| atom | 1179 | 0 | ILE | 151 | | 38.599 | | | 1.00 19.71 | | AAAA |
| ATOM | 1180 | | GLU | 152 152 | | 39.434 | | 58.533 | 1.00 13.85 | | AAAA |
| ATOM | 1181 | | GLU | 152 | | 39.362 | | | 1.00 20.21 | | AAAA |
| ATOM | 1182 | | GLU | 152 153 | | 38.033 | | | 1.00 22.16 | | AAAA |
| ATOM | 1183 | | GLU | 152 152 | | 37.83 | | | 1.00 26.94 | | AAAA |
| ATCM | 1184 | | | 152 152 | | 36.720 | | | 1.00 25.03 | | AAAA |
| atom | 1185 | | 1 GLU | | | 38.80 | | | 3 1.00 24.95 | | AAAA |
| atom | 1186 | | 2 GLU | 152 152 | | 40.86 | | • | 2 1.00 16.85 | • | AAAA |
| ATOM | 1187 | | GLU | 152 | | 41.62 | | | | | AAAA |
| ATOM | 1188 | 0 | GLU | 134 | | | _ . | • | | | • |
| | | | | | | | | | | | |

| | | | | | | - | | | | |
|--------|------|------|--------|-----|---|-----------|---------|----------|------------|------|
| | | | | | | 41.228 | 21.290 | 58.931 | 1.00 14.74 | AAAA |
| MOTA | 1189 | N | TYR | 153 | | | 21.672 | 59.350 | 1.00 17.71 | AAAA |
| ATOM | 1190 | CA | ΤΫ́R | 153 | | 42.574 | | | 1.00 13.26 | AAAA |
| ATOM | 1191 | CB | TYR | 153 | | 42.757 | 23.193 | | 1.00 15.20 | AAAA |
| | 1192 | ÇG | TYR | 153 | | 44.059 | 23.727 | | | |
| ATOM | | | | 153 | | 45.234 | 23.726 | | 1.00 18.41 | AAAA |
| ATOM | 1193 | | | | | 46.438 | 24.219 | 59.511 | 1.00 21.03 | AAAA |
| ATOM | 1194 | | | 153 | | 44.115 | 24.220 | 61.028 | 1.00 21.16 | AAAA |
| ATOM | 1195 | | TYR | 153 | , | | 24.705 | 61.570 | 1.00 19.76 | AAAA |
| MOTA | 1196 | CE2 | TYR | 153 | | 45.288 | | 60.824 | 1.00 25.97 | AAAA |
| ATOM | 1197 | CZ | TYR | 153 | | 46.440 | 24.711 | | 1.00 23.15 | AAAA |
| | 1198 | OH | TYR | 153 | | 47.571 | 25.235 | 61.410 | 1.00 23.13 | AAAA |
| ATOM | | C | TYR | 153 | | 42.712 | 21.274 | 60.828 | 1.00 20.00 | |
| MOTA | 1199 | | | 153 | | 43.722 | 20.698 | 61.247 | 1.00 19.61 | AAAA |
| MOTA | 1200 | 0 | TYR | | | 41.683 | 21.569 | 61.616 | 1.00 17.78 | AAAA |
| ATOM | 1201 | N | LEU | 154 | | 41.698 | 21.239 | 63.042 | 1.00 17.26 | AAAA |
| MOTA | 1202 | CA | LEU | 154 | | | 21.913 | 63.744 | 1.00 20.44 | AAAA |
| MOTA | 1203 | CB | LEU | 154 | | 40.511 | | 63.942 | 1.00 19.57 | AAAA |
| ATOM | 1204 | CG | LEU | 154 | | 40.636 | 23.434 | | 1.00 22.48 | AAAA |
| | 1205 | | LEU | 154 | | 39.277 | 24.046 | 64.309 | 1.00 22.40 | AAAA |
| ATOM | 1206 | | LEU | 154 | | 41.692 | 23.709 | 65.044 | 1.00 20.84 | AAAA |
| MOTA | | C | LEU | 154 | | 41.669 | 19.715 | 63.262 | 1.00 19.69 | |
| MOTA | 1207 | | | 154 | | 42.357 | 19.191 | 64.149 | 1.00 22.91 | AAAA |
| ATOM | 1208 | 0 | LEU | | | 40.878 | 18.996 | 62.469 | 1.00 20.88 | |
| ATOM | 1209 | N | ARG | 155 | | 40.840 | 17.539 | 62.622 | 1.00 22.64 | AAAA |
| MOTA | 1210 | CA | ARG | 155 | | | | 61.652 | 1.00 25.69 | AAAA |
| MOTA | 1211 | CB | ARG | 155 | | 39.829 | 16.905 | 61.893 | 1.00 27.64 | AAAA |
| ATOM | 1212 | CG | ARG | 155 | | 38.384 | 17.394 | | 1.00 27.67 | AAAA |
| | 1213 | CD | ARG | 155 | | 37.382 | 16.834 | 60.892 | 1.00 25.67 | AAAA |
| ATOM | | NE | ARG | 155 | | 36.931 | 15.497 | 61.246 | 1.00 30.88 | AAAA |
| MOTA | 1214 | | | 155 | | 36.135 | 14.753 | 60.488 | 1.00 36.28 | |
| MOTA | 1215 | CZ | ARG | | | 35.705 | 15.218 | 59.318 | 1.00 26.96 | AAAA |
| MOTA | 1216 | | ARG | 155 | • | 35.737 | 13.562 | 60.923 | 1.00 27.33 | AAAA |
| ATOM | 1217 | NH2 | ARG | 155 | | | 16.966 | 62.390 | 1.00 28.00 | AAAA |
| ATOM | 1218 | С | ARG | 155 | | 42.235 | | 63.119 | 1.00 28.05 | AAAA |
| ATOM | 1219 | 0 | ARG - | 155 | | 42.674 | 16.070 | 61.395 | 1.00 23.53 | AAAA |
| ATOM | 1220 | N | LYS | 156 | | 42.949 | 17.486 | | 1.00 26.79 | AAAA |
| | 1221 | CA | LYS | 156 | | 44.290 | 16.977 | 61.128 | 1.00 20.79 | AAAA |
| MOTA | | | LYS | 156 | | 44.854 | 17.558 | 59.824 | 1.00 26.01 | AAAA |
| MOTA | 1222 | CB | | 156 | | 46.213 | 16.955 | 59.444 | 1.00 29.70 | |
| MOTA | 1223 | CG | LYS | 156 | | 46.632 | 17.308 | 58.035 | 1.00 28.77 | AAAA |
| MOTA | 1224 | CD | LYS | | | 45.685 | 16.692 | 57.005 | 1.00 39.79 | AAAA |
| ATOM | 1225 | CE | LYS | 156 | | 45.671 | 15.192 | 57.058 | 1.00 36.33 | AAAA |
| ATOM | 1226 | NZ | LYS | 156 | | | 17.260 | 62.299 | 1.00 26.40 | AAAA |
| ATCM | 1227 | С | LYS | 156 | | 45.233 | | 62.529 | 1.00 26.19 | AAAA |
| MOTA | 1228 | 0 | LYS | 156 | | 46.188 | | | 1.00 22.50 | AAAA |
| | 1229 | N | LYS | 157 | | 44.960 | | | 1.00 21.12 | AAAA |
| ATOM | | CA | LYS | 157 | | 45.757 | 18.709 | | 1.00 21.12 | AAAA |
| ATOM | 1230 | | | 157 | | 45.535 | 20.181 | 64.591 | 1.00 28.95 | |
| MOTA | 1231 | CB | | 157 | | 46.160 | | 63.652 | 1.00 25.94 | AAAA |
| ATCM | 1232 | | | | | 47.669 | | | 1.00 35.16 | AAAA |
| ATOM | 1233 | CD | | 157 | | | | | 1.00 39.24 | AAAA |
| ATOM | 1234 | CE | LYS | 157 | | 48.281 | | | 1.00 40.01 | 4AAA |
| ATCM | 1235 | NZ | LYS | 157 | | 49.742 | | | | AAAA |
| ATOM | 1236 | | LYS | 157 | | 45.421 | | | | AAAA |
| | 1237 | | LYS | 157 | | 46.085 | | | | AAAA |
| ATCM | | | GLY | 158 | | 44.392 | 16.995 | 65.284 | | AAAA |
| ATCM | 1238 | | | 158 | | 44.023 | | 66.376 | 1.00 24.82 | |
| ATOM: | 1239 | | | | | 42.771 | | | 1.00 33.13 | AAAA |
| ATCM | 1240 |) C | GLY | 158 | | 42.421 | | | | AAAA |
| MOTA | 1241 | . 0 | GLY | 158 | | 42.421 | | | | AAAA |
| ATCM | 1242 | N | PHE | 159 | | 42.085 | | | | AAAA |
| ATOM | 1243 | CA | PHE | 159 | | 40.866 | | | | AAAA |
| | 1244 | | | 159 | | 40.410 | | 67.186 | | AAAA |
| MOTA | 1245 | | | 159 | | 41.264 | 20.343 | 3 67.827 | | AAAA |
| ATOM | | | | 159 | | 42.439 | 20.78 | 5 67.220 | | |
| ATOM | | | 1 PHE | | | 40.920 | | 2 69.076 | 1.00 21.10 | AAAA |
| ATOM | | | 2 PHE | 159 | | 43.26 | | | 1.00 26.24 | AAAA |
| ATCM | 1248 | B CE | E1 PHE | 159 | | | | | | AAAA |
| ATCM | | | 2 PHE | 159 | | 41.73 | | | | AAAA |
| ATCM | | | | 159 | | 42.90 | | | | AAAA |
| | | | PHE | 159 | | 39.79 | | | | AAAA |
| ATOM | | | PHE | 159 | | 39.63 | 9 16.53 | | | AAAA |
| ATCM | | | | 160 | | 39.05 | | | | AAAA |
| · ATCM | | | | | | 38.01 | | | 1.00 24.26 | AAAA |
| ATOM | 125 | 4 C | A LYS | 160 | | ۵۰۰۰۰ بار | | - | | • |
| | • | | • | | | | | | | • |
| | | | | | | | | | | |

| A COM | 1255 | СВ | LYS | 160 | 38 | .360 | 14.098 | 68.668 | 1.00 | 22.86 | AAAA |
|-------|------|-----|-----|-------|----|------------------|--------|--------|--------|---------|--------|
| MOTA | 1256 | | LYS | 160 | 39 | .625 | 13.424 | 68.157 | | 43.16 | AAAA |
| MOTA | 1257 | | LYS | 160 | | .222 | 12.417 | 69.141 | | 54.05 | AAAA |
| MOTA | | | LYS | 160 | - | .236 | 11.343 | 69.577 | | 62,87 | AAAA |
| MOTA | 1258 | | LYS | 160 | | .154 | 11.890 | 70.446 | 1.00 | 68.11 | AAAA |
| ATOM | 1259 | | | 160 | | .599 | 15.822 | 68.225 | 1.00 | 21.12 | AAAA |
| ATOM- | 1260 | | LYS | 160 | | .632 | 15.072 | 68.051 | 1.00 | 22.43 | AAAA |
| ATOM | 1261 | | LYS | | | .476 | 17.042 | 68.733 | 1.00 | 19.68 | AAAA |
| ATOM | 1262 | | ARG | 161 | | | 17.594 | 69.073 | | 20.84 | AAAA |
| ATOM | 1263 | | ARG | .161 | | .164 | 17.467 | 70.572 | | 26.02 | AAAA |
| MOTA | 1264 | CB | ARG | 161 | | .865 | 16.031 | 71.080 | | 28.47 | AAAA |
| MOTA | 1265 | CG | ARG | 161 | | .715 | | 72.523 | | 30.38 | AAAA |
| ATOM | 1266 | CD | ARG | 161 | | .213 | 16.025 | 73.445 | | 32.99 | AAAA |
| MOTA | 1267 | NE | ARG | 161 | | .098 | 16.734 | 73.883 | | 40.49 | AAAA |
| ATOM | 1268 | CZ | ARG | 161 | | .272 | 16.278 | | | 31.49 | AAAA |
| MOTA | 1269 | NH1 | | 161 | | .724 | 15.094 | 73.489 | | 38.54 | - AAAA |
| ATOM | 1270 | NH2 | ARG | 161 | | .003 | 17.014 | 74.712 | | 18.98 | AAAA |
| ATOM | 1271 | С | ARG | 161 . | | .171 | 19.060 | 68.680 | | 23.57 | AAAA |
| ATOM | 1272 | 0 | ARG | 161 | | .552 | 19.932 | 69.460 | | | AAAA |
| ATOM | 1273 | N | ILE | 162 | | .743 | 19.332 | 67.458 | | 19.82 | AAAA |
| ATOM | 1274 | CA | ILE | 162 | | .744 | 20.700 | 66.947 | | 17.81 | AAAA |
| ATOM | 1275 | CB | ILE | 162 | | .522 | 20.717 | 65.626 | | 18.33 | |
| ATOM | 1276 | | ILE | 162 | 35 | .542 | 22.110 | 65.042 | | 13.65 | AAAA |
| ATOM | 1277 | | ILE | 162 | 36 | .937 | 20,200 | 65.895 | | 18.15 | AAAA |
| | 1278 | | ILE | 162 | 37 | .722 | 19.852 | 64.670 | | 22.52 | AAAA |
| MOTA | 1279 | C | ILE | 162 | 33 | .316 | 21.184 | 66.724 | | 14.71 | AAAA |
| MOTA | 1280 | Ö | ILE | 162 | 32 | .520 | 20.492 | 66.126 | | 17.99 | AAAA |
| MOTA | 1281 | Ŋ | LEU | 163 | | .996 | 22.374 | 67.217 | | 16.93 | AAAA |
| MOTA | 1281 | CA | LEU | 163 | | .653 | 22.902 | 67.061 | | 20.73 | AAAA |
| MOTA | _ | CB | LEU | 163 | | 115 | 23.376 | 68.421 | | 18.45 | AAAA |
| ATOM | 1283 | CG | LEU | 163 | | .846 | 24.236 | 68.463 | . 1.00 | 19.99 | AAAA |
| ATOM | 1284 | | LEU | 163 | | 3.657 | 23.408 | 67.975 | 1.00 | 15.66 | AAAA |
| MOTA | 1285 | | LEU | 163 | | .609 | 24.751 | 69.870 | | 18.74 | AAAA |
| ATOM | 1286 | | LEU | 163 | | .705 | 24.071 | 66.106 | | 18.40 | AAAA |
| ATOM | 1287 | С | | 163 | | 2.607 | 24.889 | 66.188 | | 18.65 | AAAA |
| MOTA | 1288 | 0 | LEU | 164 | | 752 | 24.128 | 65.186 | 1.00 | 16.97 | AAAA |
| ATOM | 1289 | N | TYR | 164 | | 0.656 | 25.246 | 64.252 | 1.00 | 11.76 | AAAA |
| MOTA | 1290 | CA | TYR | 164 | | 7.782 | 24.754 | 62.816 | 1.00 | 14.07 | AAAA |
| MOTA | 1291 | CB | TYR | 164 | | 5.593 | 25.851 | 61.797 | 1.00 | 14.51 | AAAA |
| ATOM | 1292 | CG | TYR | 164 | | 1.573 | 26.822 | 61.562 | | 27.08 | AAAA |
| MOTA | 1293 | | TYR | 164 | | 1.353 | 27.832 | 60.598 | 1.00 | 26.21 | AAAA |
| MOTA | 1294 | CE1 | | 164 | | 9.415 | 25.916 | 61.070 | 1.00 | 0 21.45 | AAAA |
| MOTA | 1295 | CD2 | | | | 9.193 | 26.891 | 60.137 | | 0 21.89 | AAAA |
| MOTA | 1296 | CE2 | | 164 | | 0.148 | 27.839 | 59.896 | | 0 16.35 | AAAA |
| MOTA | 1297 | cz | TYR | 164 | | 9.857 | 28.764 | 58.913 | | 0 27.44 | AAAA |
| ATOM | 1298 | OH | TYR | 164 | 2: | 9.279 | 25.873 | 64.463 | | 0 15.67 | AAAA |
| ATOM | 1299 | С | TYR | 164 | | | 25.177 | 64.455 | 1.0 | 0 16.07 | AAAA |
| MOTA | 1300 | 0 | TYR | 164 | | 8. ⁶⁰ | 27.187 | 64.674 | 1.0 | 0 14.52 | AAAA |
| MOTA | 1301 | Ŋ | ILE | 165 | | | 27.887 | | 1.0 | 0 18.37 | AAAA |
| ATOM | 1302 | CA | ILE | 165 | | 7.:78 | 28.596 | | 1.0 | 0 13.31 | AAAA |
| MOTA | 1303 | CB | ILE | 165 | | 7.959 | 29.359 | | | 0 13.06 | AAAA |
| MOTA | 1304 | | ILE | 165 | | 6.654 | 27.573 | 67.376 | | 0 17.28 | AAAA |
| ATOM | 1305 | | ILE | 165 | | 8.172 | | | | 0 15.02 | AAAA |
| MOTA | 1306 | CD1 | ILE | 165 | | 8.493 | 28.209 | | 1 0 | 0 20.75 | AAAA |
| MOTA | 1307 | С | ILE | 165 | | 7.853 | 28.926 | | 1.0 | 0 16.67 | AAAA |
| MOTA | 1308 | 0 | ILE | 165 | | 8.759 | | | | 0 15.37 | AAAA |
| MOTA | 1309 | N | ASP | 166 | | 6.725 | | | | 0 15.63 | AAAA |
| MOTA | 1310 | CA | ASP | 166 | | 6.503 | | | | 0 12.31 | AAAA |
| ATOM | 1311 | CB | ASP | 166 | | 6.276 | 28.885 | | | 0 12.31 | AAAA |
| ATOM | 1312 | CG | ASP | 166 | | 6.279 | | 59.393 | | 0 16.37 | AAAA |
| ATOM | 1313 | | ASP | 166 | 2 | 5.378 | 30.508 | | | 0 13.41 | AAAA |
| ATOM | 1314 | | ASP | 166 | | 7.187 | | | | 0 16.06 | AAAA |
| | 1315 | 3 | ASP | 166 | 2 | 5.334 | 30.740 | | | 0 15.54 | |
| ATOM | 1316 | | ASP | 166 | 2 | 4.160 | 30.355 | | | 0 12.60 | AAAA |
| MOTA | 1317 | | LEU | 167 | | 5.647 | | | | 0 14.02 | AAAA |
| MOTA | 1317 | | LEU | 167 | | 4.598 | 32.993 | | | 0 12.05 | AAAA |
| ATOM | 1319 | | | | | 5.051 | | 63.767 | | 0 14.61 | AAAA |
| ATOM | 1319 | | LEU | | | 5.345 | | | 1.0 | 0 17.20 | AAAA |
| ATCM | 1320 | | | | _ | | | • | | | • |

| | | CD1 | T E:1 | 167 | 25.635 | 34.271 | | 1.00 28.82 | AAAA |
|--------------|--------------|---------------|--------------|------------|------------------|---------------------------------------|------------------|----------------------------|--------------|
| MOTA | 1321 1322 | CD2 | | 167 | 24.148 | 32.372 | | 1.00 18.59 | AAAA |
| MOTA | | | LEU | 167 | 24.122 | 33.776 | | 1.00 12.62 | AAAA AAAA |
| ATOM ATOM | 1324 | | LEU | 167 | 23.288 | 34.678 | | 1.00 15.00 1.00 14.35 | AAAA |
| ATOM | 1325 | | ASP | 168 | 24.667 | 33.431 | | 1.00 14.33 | AAAA |
| ATOM | 1326 | | ASP | 168 | 24.277 | 34.056 | | 1.00 25.15 | AAAA |
| MOTA | | | ASP | 168 | 25.060 | 33.409 | 57.880 56.573 | 1.00 48.45 | AAAA |
| ATOM | 1328 | CG | ASP | 168 | 24.908 | 34.145 | | 1.00 54.45 | AAAA |
| ATOM | 1329 | OD1 | | 168 | 25.477 | 35.247 33.633 | 55.668 | 1.00 44.71 | AAAA |
| ATOM | 1330 | OD2 | | 168 | 24.215 22.787 | 33.751 | 58.834 | 1.00 16.30 | AAAA |
| MOTA | 1331 | С | ASP | 168 | 22.787 | 32.696 | 59.252 | 1.00 17.72 | AAAA |
| MOTA | 1332 | 0 | ASP | 168 169 | 22.059 | 34.657 | 58.175 | 1.00 14.11 | AAAA |
| MOTA | 1333 | N | ALA ALA | 169 | 20.618 | 34.503 | 57.934 | 1.00 19.61 | AAAA |
| MOTA | 1334 | CA CB | ALA | 169 | 20.006 | 35.856 | 57.470 | 1.00 13.56 | AAAA |
| MOTA | 1335 1336 | C | ALA | 169 | 20.277 | 33.400 | 56.926 | 1.00 18.23 | AAAA AAAA |
| MOTA MOTA | 1337 | Ö | ALA | 169 | 19.105 | 33.159 | 56.641 | 1.00 17.20 | AAAA |
| ATOM | 1338 | N | HIS | 170 | 21.301 | | 56.373 | 1.00 16.53 1.00 17.51 | AAAA |
| ATOM | 1339 | CA | HIS | 170 | 21.075 | | 55.436 | 1.00 17.31 | AAAA |
| ATOM | 1340 | CB | HIS | 170 | 21.616 | | 54.033 53.377 | 1.00 25.38 | AAAA |
| ATOM | 1341 | CG | HIS | 170 | 20.954 | | 52.487 | 1.00 19.33 | AAAA |
| ATOM | 1342 | | HIS | 170 | 19.934 21.308 | | 53.638 | 1.00 18.17 | AAAA |
| ATOM | 1343 | | HIS | 170 | 20.535 | | 52.935 | 1.00 30.34 | AAAA |
| ATOM | 1344 | | HIS | 170 170 | 19.692 | | 52.229 | 1.00 17.51 | AAAA |
| MOTA | 1345 | | HIS | 170 | 21.781 | · · · · · · · · · · · · · · · · · · · | 55.967 | 1.00 16.72 | AAAA |
| MOTA | 1346 | C | HIS HIS | 170 | 22.827 | | 56.610 | 1.00 15.92 | AAAA |
| ATOM | 1347 | и О | HIS | 171 | 21.209 | | 55.682 | 1.00 15.28 | AAAA AAAA |
| MOTA | 1348 1349 | CA | HIS | 171 | 21.75 | | 56.123 | 1.00 12.53 | AAAA |
| MOTA MOTA | 1350 | CB | HIS | 171 | 20.702 | 26.878 | 55.814 | 1.00 14.09 1.00 17.27 | AAAA |
| MOTA | 1351 | ĊĞ | HIS | 171 | 21.180 | | 55.980 55.090 | 1.00 17.27 | AAAA |
| MOTA | 1352 | | HIS | 171 | 21.249 | | 57.181 | 1.00 26.73 | AAAA |
| ATOM | 1353 | | HIS | 171 | 21.622 | | 57.021 | 1.00 15.98 | AAAA |
| ATOM | 1354 | | HIS | 171 . | 21.945 21.725 | - | 55.761 | 1.00 20.03 | AAAA |
| MOTA | 1355 | | HIS | 171 | 23.10 | | | 1.00 15.55 | AAAA |
| ATOM | 1356 | C | HIS | 171 171 | 23.31 | | | 1.00 17.03 | AAAA |
| MOTA | 1357 | 0 | HIS CYS | 172 | 24.02 | | 56.323 | 1.00 14.33 | AAAA AAAA |
| ATOM | 1358 1359 | N CA | CYS | 172 | 25.35 | | 55.866 | 1.00 13.65 | AAAA |
| ATOM | 1360 | CB | CYS | 172 | 26.33 | 0 26.631 | | 1.00 12.99 1.00 17.17 | AAAA |
| MOTA MOTA | 1361 | SG | CYS | 172 | 25.68 | | | 1.00 17.17 | AAAA |
| ATOM | 1362 | С | CYS | 172 | 25.21 | | | 1.00 14.95 | AAAA |
| ATOM | 1363 | 0 | CYS | 172 | 25.75 | | | 1.00 15.42 | AAAA |
| ATOM | 1364 | N | ASP | 173 | 24.51 24.30 | | | 1.00 14.75 | AAAA: |
| MOTA | 1365 | CA | ASP | 173 | 23.33 | | | 1.00 17.73 | AAAA |
| MOTA | 1366 | CB | ASP | 173 173 | 23.76 | 5 24.966 | | 1.00 22.84 | AAAA |
| MOTA | 1367 | CG | ASP 1 ASP | 173 | 23.10 | | 3 50.216 | | AAAA |
| MOTA | 1368 | | 2 ASP | 173 | 24.73 | 0 25.728 | 3 51.504 | | AAAA AAAA |
| ATOM | 1369 1370 | C C | ASP | 173 | 25.59 | 0 23.145 | | | AAAA |
| ATOM ATOM | 1371 | Ö | ASP | 173 | 25.68 | | | | AAAA |
| MOTA | 1372 | | GLY | 174 | 26.58 | | | | AAAA |
| ATOM | 1373 | | | 174 | 27.86 | | | | AAAA |
| MOTA | 1374 | | GLY | 174 | 28.50 | 8 22.72 | | 4- 40 | AAAA |
| ATOM | 1375 | 0 | GLY | 174 | 28.97 | | | | AAAA |
| ATOM | 1376 | N | VAL | 175 | 28.55 29.13 | | · | 1.00 16.54 | AAAA |
| ATOM | | | | 175 175 | 29.13 | | | 1.00 15.88 | AAAA |
| MOTA | 1378 | CB | | 175 175 | 29.9 | | 7 58.307 | 1.00 15.35 | AAAA |
| ATOM | | | 1 VAL | 175 175 | 29.9 | | 8 56.476 | | AAAA |
| ATOM | | | 2 VAL VAL | 175 | 28.3 | 18 21.72 | 0 56.467 | | AAAA AAAA |
| MOTA | | | VAL | 175 | 28.8 | 76 20. 7 3 | | | AAAA |
| ATOM | | _ | GLN | 176 | 26.9 | 96 21.79 | | 1.00 17.74 2 1.00 15.66 | AAAA |
| MOTA MOTA | | | | 176 | 26.1 | 64 20.68 | | | AAAA |
| ATOM ATOM | | | | 176 | 24.6 | | | | AAAA |
| ATOM | | | | 176 | 23.7 | 89 19.78 | 5 30.33 | 2 1,00 1 | • |
| 7100 | | | | | | | | | |

| | 1307 | CD G | LN | 176 | 22.325 | 20.106 | | 1.00 21.52 | AAAA |
|--------------|--------------|------|------------|-----|--------|----------|----------|--------------------------|--------------|
| MOTA | 1387 | OE1 | | 176 | 21.850 | 21.016 | 57.567 | 1.00 21.72 | AAAA |
| ATOM | 1388 | | SLN | 176 | 21.581 | 19.348 | 56.064 | 1.00 20.30 | AAAA |
| MOTA | 1389 | | SLN | 176 | 26.527 | 19.387 | 56.121 | 1.00 16.33 | AAAA |
| MOTA | 1390 | | SLN | 176 | 26.751 | 18.354 | 56.748 | 1.00 17.46 | AAAA |
| MOTA | 1391 | _ | GLU | 177 | 26.581 | 19.443 | 54.799 | 1.00 22.24 | AAAA . |
| MOTA | 1392 | | GLU | 177 | 26.909 | 18.251 | 54.021 | 1.00 19.67 | AAAA |
| ATOM | 1393 | | 3LU 3LU | 177 | 26.857 | 18.587 | 52.533 | 1.00 15.55 | AAAA |
| MOTA | 1394 | | GLU | 177 | 27.131 | 17.388 | 51.623 | 1.00 20.24 | AAAA |
| MOTA | 1395 | | GLU | 177 | 26.960 | 17.740 | 50.159 | 1.00 27.00 | AAAA |
| ATOM | 1396 | OE1 | | 177 | 27.974 | 17.935 | 49.450 | 1.00 30.23 | AAAA |
| MOTA | 1397 | | GLU | 177 | 25.796 | 17.853 | 49.725 | 1.00 26.89 | AAAA |
| MOTA | 1398 | | GLU | 177 | 28.284 | 17.713 | 54.376 | 1.00 20.42 | AAAA |
| MOTA | 1399 | | GLU | 177 | 28.486 | 16.503 | 54.527 | 1.00 17.05 | AAAA |
| ATOM | 1400 | _ | ALA | 178 | 29.233 | 18.626 | 54.527 | 1.00 19.67 | AAAA |
| MOTA | 1401 | | ALA | 178 | 30.611 | 18.259 | 54.839 | 1.00 18.18 | AAAA |
| ATOM | 1402 | | ALA | 178 | 31.464 | 19.519 | 54.918 | 1.00 12.76 | AAAA |
| MOTA | 1403 | - | ALA | 178 | 30.806 | 17.418 | 56.106 | 1.00 17.56 | AAAA |
| MOTA | 1404 | _ | ALA | 178 | 31.690 | 16.555 | 56.167 | 1.00 17.72 | AAAA |
| MOTA | 1405 | | PHE | 179 | 29.981 | 17.656 | 57.116 | 1.00 18.82 | AAAA |
| ATOM | 1406 | | PHE | 179 | 30.124 | 16.945 | 58.379 | 1.00 20.26 | AAAA |
| MOTA | 1407 | | PHE | 179 | 30.554 | 17.948 | 59.439 | 1.00 13.17 | AAAA |
| MOTA | 1408 | | PHE | 179 | 31.779 | 18.693 | 59.048 | 1.00 16.28 | AAAA |
| MOTA | 1409 | | | 179 | 31.705 | 20.017 | 58.610 | 1.00 13.77 | AAAA |
| MOTA | 1410 | CD1 | PHE | 179 | 33.002 | 18.031 | 58.995 | 1.00 15.57 | AAAA |
| MOTA | 1411 | | PHE | 179 | 32.845 | | 58.114 | 1.00 20.03 | AAAA |
| MOTA | 1412 | | PHE | 179 | 34.145 | | 58.500 | 1.00 20.30 | AAAA |
| MOTA | 1413 | | PHE | 179 | 34.060 | 20.002 | 58.058 | 1.00 19.51 | AAAA |
| MOTA | 1414 | | PHE | 179 | 28.882 | | 58.833 | 1.00 18.52 | AAAA |
| ATOM | 1415 | 0 | PHE | 179 | 28.773 | 15.828 | 60.000 | 1.00 20.21 | AAAA |
| MOTA | 1416 | N | TYR | 180 | 27.969 | 16.016 | 57.895 | 1.00 18.33 | AAAA |
| ATOM | 1417 | CA | TYR | 180 | 26.698 | 15.379 | 58.176 | 1.00 19.93 | AAAA |
| MOTA | 1418 1419 | CB | TYR | 180 | 25.874 | | 56.894 | 1.00 20.97 | AAAA |
| MOTA | 1419 | CG | TYR | 180 | 24.402 | 15.341 | 57.159 | 1.00 19.80 | AAAA |
| MOTA | 1421 | | TYR | 180 | 23.565 | 14.337 | 56.686 | 1.00 23.87 | AAAA |
| ATOM | 1421 | | TYR | 180 | 22.203 | | 56.898 | 1.00 21.32 | AAAA AAAA |
| ATOM | 1423 | CD2 | TYR | 180 | 23.831 | 16.416 | 57.865 | 1.00 19.02 | AAAA |
| MOTA | 1424 | CE2 | TYR | 180 | 22.470 | | 58.084 | 1.00 26.84 | AAAA |
| ATOM | 1425 | CZ | TYR | 180 | 21.659 | | 57.594 | 1.00 30.54 | AAAA |
| MOTA | 1426 | он | TYR | 180 | 20.310 | 15.514 | 57.794 | 1.00 22.81 | AAAA |
| ATOM | 1427 | c. | TYR | 180 | 26.85 | | 58.737 | 1.00 22.61 | AAAA |
| MOTA MOTA | 1428 | ŏ | TYR | 180 | 26.06 | | 59.579 | 1.00 23.44 | AAAA |
| ATOM | 1429 | N | ASP | 181 | 27.89 | | 58.253 | 1.00 22.27 | AAAA |
| MOTA | 1430 | CA | ASP | 181 | 28.24 | | 58.590 | 1.00 33.84 1.00 41.74 | AAAA |
| MOTA | 1431 | CB | ASP | 181 | 28.91 | | 57.339 | 1.00 41.74 | AAAA |
| ATOM | 1432 | CG | ASP | 181 | 30.03 | 5 10.363 | | 1.00 57.71 | AAAA |
| MOTA | 1433 | | ASP | 181 | 30.99 | 10.780 | | 1.00 65.77 | AAAA |
| ATOM | 1434 | OD2 | ASP | 181 | 29.96 | | | 1.00 33.77 | AAAA |
| ATOM | 1435 | C | ASP | 181 | 29.10 | | | 1.00 30.21 | AAAA |
| ATOM | 1436 | О | ASP | 181 | 29.30 | | 60.227 | | AAAA |
| ATOM | 1437 | N | THR | 182 | 29.61 | 5 12.696 | | 1.00 21.19 | AAAA |
| MOTA | 1438 | CA | THR | 182 | 30.47 | 2 12.466 | | | AAAA |
| ATOM | 1439 | СВ | THR | 182 | 31.91 | 8 12.977 | | | AAAA |
| ATOM | 1440 | | THR | 182 | 32.72 | | | | AAAA |
| MOTA | 1441 | CG2 | | 182 | 31.92 | | | | AAAA |
| MOTA | 1442 | C | THR | 182 | 30.01 | | | | AAAA |
| ATOM | 1443 | 0 | THR | 182 | 29.30 | | | | AAAA |
| ATOM | 1444 | N | ASP | 183 | 30.43 | | | | AAAA |
| ATOM | 1445 | CA | ASP | 183 | 30.08 | 6 12.894 | | | AAAA |
| ATOM | 1446 | | ASP | 183 | 29.73 | | | | AAAA |
| ATOM | 1447 | | ASP | 183 | 30.92 | | | | AAAA |
| MOTA | 1448 | | ASP | 183 | 31.66 | 7 10.502 | | | AAAA |
| MOTA | 1449 | | ASP | 183 | 31.09 | 5 10.32 | | | AAAA |
| ATOM | 1450 | | ASP | 183 | 31.25 | 7 13.68 | | | AAAA |
| ATOM | 1451 | | ASP | 183 | 31.23 | 6 14.09 | | | AAAA |
| ATOM | | | GLN | 184 | 32.28 | 13.90 | 9 65.131 | 1.00 21.00 | • |
| ALOM | | | | • | | | | | |

| | | | | | ٠ | | | | | |
|--------------|---------------|--------|------------|------------|----|------------------|--------------------|------------------|--------------------------|------------------|
| | | CN C1 | LN | 184 | | 33.437 | | | 1.00 17.65 | AAAA |
| MOTA | | | LN | 184 | | | | | 1.00 21.36 | AAAA AAAA |
| ATOM | 1454 1455 | | LN | 184 | | | | | 1.00 27.38 1.00 31.96 | AAAA |
| MOTA MOTA | 1456 | | LN | 184 | | • • • • • | | | 1.00 31.90 | AAAA |
| ATOM | 1457 | OE1 G | | 184 | | - | 12.760 | | 1.00 23.30 | AAAA |
| ATOM | 1458 | NE2 G | | 184 | | 37.239 | 11.878 | | 1.00 18.54 | AAAA |
| ATOM | 1459 | C G | LN | 184 | ٠. | 33.207 | 16.165 17.009 | 65.972 | 1.00 18.11 | AAAA |
| ATOM | 1460 | | LN. | 184 | | 33.881 | 16.481 | 64.519 | 1.00 19.18 | AAAA |
| MOTA | 1461 | | AL | 185 | | 32.258 31.934 | 17.872 | 64.267 | 1.00 21.57 | AAAA |
| MOTA | 1462 | | AL | 185 | | 32.261 | 18.264 | 62.807 | 1.00 22.64 | AAAA |
| MOTA | 1463 | | AL | 185 185 | • | 31.994 | 19.768 | 62.591 | 1.00 16.26 | AAAA |
| MOTA | 1464 | CG1 V | | 185 | | 33.722 | 17.924 | 62.500 | 1.00 16.77 | AAAA |
| MOTA | 1465 | CG2 V | AL | 185 | | 30.449 | 18.035 | 64.523 | 1.00 16.91 | AAAA AAAA |
| MOTA | 1466 | _ | AL | 185 | | 29.658 | 17.156 | 64.179 | 1.00 20.79 | AAAA |
| MOTA | 1467 1468 | - | HE. | 186 | | 30.081 | 19.146 | 65.153 | 1.00 18.73 1.00 16.22 | AAAA |
| ATOM ATOM | 1469 | | HE | 186 | | 28.687 | 19.446 | 65.435 | 1.00 16.22 | AAAA |
| ATOM | 1470 | | HE | 186 | | 28.432 | 19.559 | 66.952 67.299 | 1.00 17.96 | AAAA |
| ATOM | 1471 | CG E | PHE | 186 | | 26.976 | 19.682 | 67.968 | 1.00 23.24 | AAAA |
| ATOM | 1472 | CD1 F | | 186 | | 26.319 | 18.656 20.797 | 66.904 | 1.00 15.41 | AAAA |
| MOTA | 1473 | CD2 F | | 186 | | 26.240 24.953 | 18.738 | 68.235 | 1.00 18.99 | AAAA |
| MOTA | 1474 | CE1 I | | 186 | | 24.955 | 20.887 | 67.168 | 1.00 24.05 | AAAA |
| ATOM | 1475 | | PHE | 186 | | 24.234 | 19.846 | 67.838 | 1.00 22.93 | AAAA |
| MOTA | 1476 | | PHE | 186 186 | | 28.437 | 20.789 | 64.778 | 1.00 17.16 | AAAA |
| MOTA | 1477 . | | PHE PHE | 186 | | 29.192 | 21.725 | 64.993 | 1.00 19.37 | аааа аааа |
| ATOM | 1478 | - | VAL | 187 | | 27.391 | 20.874 | 63.961 | 1.00 19.67 | AAAA |
| MOTA | 1479 ·1480 | | VAL | 187 | | 27.075 | 22.116 | 63.277 | 1.00 17.74 1.00 18.65 | AAAA |
| ATOM | 1481 | | VAL | 187 | | 27.010 | 21.914 | 61.720 | 1.00 18.03 | AAAA |
| ATOM ATOM | 1482 | CG1 | | 187 | | 26.578 | 23.211 | 61.024 61.194 | 1.00 16.65 | AAAA |
| MOTA | 1483 | CG2 | | 187 | | 28.359 | 21.453 22.637 | 63.746 | 1.00 18.46 | AAAA |
| ATOM | 1484 | - | VAL | 187 | | 25.732 24.752 | 21.903 | 63.764 | 1.00 20.64 | AAAA |
| ATOM | 1485 | _ | VAL | 187 | | 25.708 | 23.899 | 64.150 | 1.00 14.42 | AAAA |
| MOTA | 1486 | | LEU | 188 188 | | 24.482 | 24.563 | 64.567 | 1.00 16.68 | AAAA |
| MOTA | 1487 | | LEU | 188 | | 24.568 | 25.070 | 66.009 | 1.00 13.98 | ААҚА АААА |
| MOTA | 1488 | | LEU LEU | 188 | | 23.522 | 26.119 | 66.450 | 1.00 13.66 | AAAA |
| MOTA | 1489 1490 | CD1 | | 188 | | 22.103 | 25.556 | 66.401 | 1.00 15.55 1.00 16.40 | AAAA |
| MOTA MOTA | 1491 | CD2 | | 188 | | 23.844 | 26.585 | 67.861 | 1.00 20.01 | AAAA |
| ATOM | 1492 | c | LEU | 188 | | 24.272 | 25.756 | 63.667 63.506 | 1.00 18.86 | AAAA |
| ATOM | 1493 | 0 | LEU | 188 | | 25.164 | 26.595 25.845 | 63.057 | 1.00 14.46 | AAAA |
| ATOM | 1494 | N | SER | 189 | | 23.106 | 27.011 | 62.230 | 1.00 14.56 | AAAA |
| ATOM | 1495 | CA | SER | 189 | | 22.841 22.896 | 26.668 | | 1.00 15.55 | AAAA |
| ATOM | 1496 | CB | SER | 189 189 | | 22.619 | 27.851 | | 1.00 14.09 | AAAA |
| MOTA | 1497 | oG | SER | 189 | | 21.487 | 27.606 | 62.508 | | AAAA AAAA |
| MOTA | 1498 | C | SER SER | 189 | | 20.509 | 26.885 | 62.578 | | |
| MOTA | 1499 1500 | 0 N | LEU | 190 | | 21.423 | 28.921 | | 1.00 14.92 | |
| ATOM | 1500 | CA | LEU | 190 | | 20.128 | 29.572 | | | |
| ATOM ATOM | 1502 | | LEU | 190 | | 20.084 | 30.663 | | | |
| ATOM | 1503 | | LEU | 190 | | 20.594 | | | | AAAA |
| MOTA | 1504 | CD1 | LEU | 190 | | 19.736 | | | | AAAA |
| ATOM | 1505 | CD2 | LEU | 190 | | 20.547 | | | | AAAA |
| ATOM | 1506 | С | LEU | 190 | | 20.035 21.031 | | | 1.00 15.43 | AAAA |
| MOTA | 1507 | | LEU | 190 | | 18.855 | | | 5 1.00 16.88 | AAAA |
| MOTA | 1508 | | HIS | 191 | | 18.732 | | | 5 1.00 14.34 | AAAA |
| ATOM | | | HIS | 191 191 | | 19.506 | | 5 58.539 | | AAAA 1 AAAA 7 |
| ATOM | | | HIS HIS | 191 | | 19.229 | 28.54 | 58.69 | | |
| ATOM | | | HIS | 191 | | 19.94 | 27.578 | g 59.319 | | ="" |
| ATOM | | | HIS | 191 | | 18.07 | 3 27.94 | | | |
| ATOM | | | HIS | 191 | | 18.08 | | | | • |
| ATOM ATOM | | NE2 | HIS | 191 | | 19.21 | | | | • |
| ATOM | | | HIS | 191 | | 17.27 | | | | 3 AAAA |
| ATOM | | | HIS | 191 | | 16.38 17.04 | 1 30.48 4 31.79 | _ | | AAAA 8 |
| ATCM | | в и | GLN | 192 | | 17.04 | - 31./3 | | | • |
| | | | | | | | | | | |

| | | | | | | 31.968 | 57.516 | 1.00 16.33 | AAAA |
|--------|--------------|-----------|------------|-------------|--------|----------|----------|--------------------------|--------------|
| MOTA | 1519 | CA (| GLN | 192 | 15.683 | | 56.283 | 1.00 17.07 | AAAA |
| ATOM | | CB (| GLN | 192 | 15.669 | 32.871 | 56.498 | .00 18.15 | AAAA |
| ATOM | | | GLN | 192 | 16.174 | 34.270 | 55.177 | 1.00 14.74 | AAAA |
| MOTA | | CD | GLN | 192 | 16.408 | 34.965 | | 1.00 20.46 | AAAA |
| ATOM | | | GLN | 192 | 15.490 | 35.566 | 54.665 | 1.00 13.44 | AAAA |
| | | | GLN | 192 | 17.630 | 34.839 | | 1.00 15.06 | AAAA |
| ATOM - | 1525 | | GLN | 192 | 15.262 | 30.584 | • | 1.00 19.23 | AAAA |
| ATOM | 1526 | - | GLN | 192 | 16.071 | 29.843 | | 1.00 15.63 | AAAA |
| MOTA | 1527 | | SER | 193 | 14.007 | 30.223 | | 1.00 13.84 | AAAA |
| MOTA | | CA | SER | 193 | 13.561 | 28.907 | | 1.00 13.84 | AAAA |
| ATCM | 1528 1529 | CB | SER | 193 | 12.097 | 28.677 | | 1.00 17.28 | AAAA |
| ATOM | 1530 | OG | SER | 193 | 11.639 | 27.439 | 56.750 | 1.00 17.30 | AAAA |
| ATOM | | C | SER | 193 | 13.687 | 28.704 | 55.350 - | 1.00 11.80 1.00 18.44 | AAAA |
| MOTA | 1531 | 0 | SER | 193 | 13.400 | 29.601 | | 1.00 10.44 | AAAA |
| MOTA | 1532 | N | PRO | 194 | 14.103 | 27.505 | | 1.00 14.59 | AAAA |
| ATOM | 1533 | CD | PRO | 194 | 14.335 | 26.325 | | 1.00 19.22 | AAAA |
| ATOM | 1534 | CA | PRO | 194 | 14.268 | 27.143 | | 1.00 15.30 | AAAA |
| MOTA | 1535 | | PRO | 194 | 14.892 | 25.737 | 53.573 | 1.00 18.33 | AAAA |
| ATOM | 1536 | CB CG | PRO | 194 | 15.359 | 25.587 | 55.007 | 1.00 22.34 | AAAA |
| MOTA | 1537 | | PRO | 194 | 12.880 | 27.104 | 52.866 | 1.00 16.40 | AAAA |
| ATOM | 1538 | C | PRO | 194 | 12.757 | 27.003 | 51.640 | 1.00 19.43 | AAAA |
| MOTA | 1539 | 0 | GLU | 195 | 11.828 | 27.151 | 53.681 | 1.00 20.57 | AAAA |
| MOTA | 1540 | N | GLU | 195 | 10.483 | 27.161 | 53.099 | 1.00 30.15 | AAAA |
| MOTA | 1541 | CA | GLU | 195 | 9.386 | 27.037 | 54.173 | 1.00 31.91 | AAAA |
| MOTA | 1542 | CB | | 195 | 8.987 | 28.325 | 54.879 | 1.00 45.60 | AAAA AAAA |
| MOTA | 1543 | CG | GLU GLU | 195 | 7.880 | 29.119 | 54.174 | 1.00 34.45 | AAAA |
| MOTA | 1544 | CD | | 195 | 7.635 | 30.259 | 54.612 | 1.00 43.98 | AAAA |
| ATOM | 1545 | OE1 | GLU | 195 | 7,241 | 28.627 | 53.210 | 1.00 38.39 | AAAA |
| MOTA | 1546 | | GLU | 195 | 10.333 | 28.474 | 52.318 | 1.00 26.92 | AAAA |
| ATOM | 1547 | C | GLU | 195 | 9.522 | 28.557 | 51.395 | 1.00 24.59 | AAAA |
| ATOM | 1548 | 0 | TYR | 196 | 11.116 | 29.501 | 52.669 | 1.00 18.16 | AAAA |
| MOTA | 1549 | N | TYR | 196 | 11.024 | 30.753 | 51.922 | 1.00 15.81 | AAAA |
| MOTA | 1550 | CA | TYR | 196 | 10.208 | 31.801 | 52.690 | 1.00 20.01 | AAAA |
| MOTA | 1551 | CB | TYR | 196 | 10.868 | 32.353 | 53.932 | 1.00 19.77 | AAAA |
| ATOM | 1552 | CG CD1 | | 196 | 11.779 | 33.408 | 53.853 | 1.00 18.24 | AAAA |
| MOTA | 1553 | CEI | | 196 | 12.407 | 33.898 | | 1.00 18.50 | AAAA |
| MOTA | 1554 | CD2 | | 196 | 10.598 | 31.801 | | 1.00 18.12 | AAAA |
| MOTA | 1555 | CE2 | | 196 | 11.223 | 32.283 | | 1.00 21.09 | AAAA |
| MOTA | 1556 | CZ | TYR | 196 | 12.125 | 33.326 | 56.235 | 1.00 20.39 | AAAA |
| MOTA | 1557 | OH | TYR | 196 | 12.759 | 33.784 | | 1.00 16.20 | AAAA |
| MOTA | 1558 | C | TYR | 196 | 12.342 | 31.372 | | 1.00 16.89 | AAAA |
| ATOM | 1559 | | TYR | 196 | 12.336 | 32.347 | | 1.00 23.08 | AAAA |
| MOTA | 1560 | C | ALA | 197 | 13.466 | 30.817 | | 1.00 17.52 | AAAA |
| MOTA | 1561 | N CA | ALA | 197 | 14.754 | 31.400 | | 1.00 20.26 1.00 20.74 | AAAA |
| ATOM | .1562 | CB | ALA | 197 | 15.315 | 32.261 | | 1.00 20.74 | AAAA |
| ATOM | 1563 | | ALA | 197 | 15.814 | 30.392 | | 1.00 13.51 | AAAA |
| ATOM | 1564 | | ALA | 197 | 15.787 | 7 29.229 | 51.457 | 1 30 19.35 | AAAA |
| ATOM | 1565 | | PHE | 198 | 16.75 | 7 30.869 | | 1 70 18.01 1.00 17.97 | AAAA |
| ATOM | 1566 | CA | | 198 | 17.86 | | | 1.00 17.37 | AAAA |
| ATOM | 1567 | | | 198 | 18.929 | 30.93 | | 1.00 20.38 | AAAA |
| MOTA | 1568 1569 | | | 198 | 20.09 | 4 30.16 | | | AAAA |
| MOTA | | | 1 PHE | 198 | 20.03 | 9 29.66 | | 1.00 29.71 | AAAA |
| ATOM | | | 2 PHE | 198 | 21.22 | 9 29.89 | | | AAAA |
| ATOM | | | 1 PHE | 198 | 21.09 | | | | AAAA |
| ATOM | | | | 198 | 22.29 | 0 29.14 | 5 48.807 | | AAAA |
| ATOM | | | | 198 | 22.21 | 8 28.64 | 6 47.493 | | AAAA |
| ATOM. | | | PHE | 198 | 18.45 | 3 29.41 | 9 51.032 | | AAAA |
| ATOM | | 5 0 | | 198 | 18.55 | 2 30.07 | | 1.00 20.95 | AAAA |
| ATOM | | | PHE PRO | 199 | 18.94 | 1 28.17 | 6 50.937 | | AAAA |
| ATOM | | | | 199 | 19.60 | 0 27.50 | 8 52.074 | | AAAA |
| ATOM | | | | 199 | 18.99 | 0 27.31 | 8 49.744 | | AAAA |
| atom | | | | 199 | 20.10 | | 4 50.095 | | AAAA |
| ATOM | | | _ | 199 | 19.81 | 3 26.08 | 51.534 | | AAAA |
| MOTA | | | PRO PRO | | 17.71 | | 5 49.312 | | AAAA |
| ATCN | | | PRO | | 17.73 | 3 25.85 | | | AAAA |
| ATO | | | PHE | | 16.62 | | 50.054 | 1.00 20.32 | |
| ATOI | 1 158 | 4 N | | | | | - | | |
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|--------------|--------------|----------|------------|------------|---|------------------|------------------|------------------|-------|--------------------|--------------|
| | 1505 | C) | PHE | 200 | • | 15.319 | 26.166 | 49.752 | 1.00 | 20.27 | AAAA |
| MOTA | 1585 1586 | | PHE | 200 | | | 26.533 | 48.346 | 1.00 | 19.77 | AAAA |
| MOTA MOTA | 1587 | | PHE | 200 | | 14.752 | 27.999 | 48.082 | 1.00 | 18.06 | AAAA |
| ATOM | 1588 | CD1 | | 200 | | | 28.644 | 47.346 | 1.00 | 18.97 | AAAA AAAA |
| MOTA | 1589 | CD2 | | 200 | | 13.00 | 28.736 | 48.519 | | 19.06 21.67 | AAAA |
| ATOM | 1590 | CE1 | | 200 | | | 30.003 | 47.042 48.221 | | 22.60 | AAAA |
| ATOM | 1591 | CE2 | | 200 | | | 30.101 30.736 | 47.482 | | 18.93 | AAAA |
| MOTA | 1592 | CZ | PHE | 200 | | | 24.637 | 49.845 | | 18.44 | AAAA |
| MOTA | 1593 | C | PHE | 200 | | 15.294 14.302 | 24.037 | 50.272 | | 20.74 | AAAA |
| MOTA | 1594 | 0 | PHE | 200 201 | | 16.384 | 24.004 | 49.418 | 1.00 | 20.77 | AAAA |
| MOTA | 1595 | N. | GLU GLU | 201 | | 16.522 | 22.542 | 49.399 | | 27.34 | AAAA |
| MOTA | 1596 1597 | CA CB | GLU | 201 | | 17.498 | 22.146 | 48.284 | | 28.99 | AAAA |
| MOTA | 1598 | CG | GLU | 201 | | 17.024 | 22.458 | 46.881 | | 34.82 | AAAA |
| ATOM ATOM | 1599 | CD | GLU | 201 | | 18.123 | 22.265 | 45.848 | 1.00 | 32.40 | AAAA AAAA |
| ATOM | 1600 | | GLU | 201 | | 18.701 | 21.155 | 45.769 | 1.00 | 38.28 40.08 | AAAA |
| MOTA | 1601 | | GLU | 201 | | 18.405 | 23.230 | 45.111 | 1.00 | 23.51 | AAAA |
| ATOM | 1602 | С | GLU | 201 | | 17.007 | 21.891 | 50.695 50.886 | 1.00 | 23.17 | AAAA |
| ATOM | 1603 | 0 | GLU | 201 | | 16.845 17.619 | 20.689 22.681 | 51.571 | 1.00 | 20.03 | AAAA |
| MOTA | 1604 | N | LYS | 202 | | 18.178 | 22.177 | 52.829 | 1.00 | 17.01 | AAAA |
| MOTA | 1605 | CA | LYS | 202 202 | | 19.666 | 21.862 | 52.634 | 1.00 | 19.24 | AAAA |
| MOTA | 1606 | CB | LYS | 202 | | 19.903 | 20.769 | 51.611 | | 36.04 | AAAA |
| MOTA | 1607 | CG CD | LYS LYS | 202 | | 20.997 | 21.162 | 50.648 | 1.00 | 45.11 | AAAA |
| MOTA | 1608 1609 | CE | LYS | 202 | | 21.060 | 20.209 | 49.463 | 1.00 | 55.83 | AAAA |
| MOTA MOTA | 1610 | NZ | LYS | 202 | | 22.024 | 20.662 | 48.422 | 1.00 | 28.09 | AAAA AAAA |
| ATOM | 1611 | С | LYS | 202 | • | | 23.240 | 53.899 | | 17.02 20.20 | AAAA |
| ATOM | 1612 | 0 | LYS | 202 | | 17.705 | 24.381 | 53.585 | 1.00 | 22.94 | AAAA |
| ATOM | 1613 | N | GLY | 203 | | 18.232 | 22.875 | 55.160 56.223 | 1 00 | 19.38 | AAAA |
| MOTA | 1614 | CA | GLY | 203 | | 18.064 16.874 | 23.850 23.564 | 57.128 | 1.00 | 20.48 | AAAA |
| MOTA | 1615 | C | GLY | 203 | | 16.607 | 24.312 | 58.070 | 1.00 | 18.55 | AAAA |
| MOTA | 1616 | 0 | GLY | 203 204 | | 16.150 | 22.484 | 56.852 | 1.00 | 15.42 | AAAA |
| MOTA | 1617 | N CA | PHE PHE | 204 | | 14.983 | 22.143 | 57.670 | 1.00 | 20.73 | AAAA |
| MOTA | 1618 1619 | CB | PHE | 204 | | 14.018 | 21.212 | 56.903 | 1.00 | 0 19.97 | AAAA AAAA |
| MOTA MOTA | 1620 | CG | PHE | 204 | | 13.441 | 21.838 | 55.667 | 1.00 | 0 19.63 | AAAA |
| ATOM | 1621 | | PHE | 204 | | 14.137 | 21.801 | 54.459 | | 0 24.96 0 18.92 | AAAA |
| ATOM | 1622 | CD2 | PHE | 204 | | 12.230 | 22.523 | 55.725 53.327 | 1 0 | 0 20.66 | AAAA |
| ATOM | 1623 | | PHE | 204 | | 13.636 11.720 | 22.438 23.169 | | 1.0 | 0 24.86 | AAAA |
| MOTA | 1624 | CE2 | | 204 | | 12.422 | 23.127 | | 1.0 | 0 23.66 | AAAA |
| MOTA | 1625 | CZ | PHE | 204 204 | | 15.376 | 21.513 | | 1.0 | 0 18.73 | AAAA |
| MOTA | 1626 | С 0 | PHE PHE | 204 | | 16.415 | 20.851 | 59.131 | 1.0 | 0 20.18 | AAAA |
| MOTA | 1627 1628 | N | LEU | 205 | | 14.518 | 21.726 | 59.994 | 1.0 | 0 19.46 | AAAA AAAA |
| ATOM ATOM | 1629 | CA | | 205 | | 14.727 | 21.244 | 61.356 | 1.0 | 0 21.09 0 23.44 | |
| ATOM | 1630 | CB | LEU | 205 | | 13.547 | 21.674 | | 1.0 | 0 23.44 | AAAA |
| MOTA | 1631 | CG | LEU | 205 | | 13.506 | 21.222 | | | 0 24.06 | AAAA |
| MOTA | 1632 | | LEU | 205 | | 14.717 | 21.736 21.743 | | _ | 0 30.63 | AAAA |
| ATOM | 1633 | | 2 LEU | 205 | | 12.224 | 19.748 | | 1.0 | 0 23.53 | AAAA |
| MOTA | 1634 | | LEU | 205 205 | | 15.659 | 19.315 | | 1.0 | 0 21.28 | AAAA |
| ATOM | 1635 | | LEU | 205 | | 14.356 | 18.959 | | 1.0 | 0 21.59 | AAAA |
| ATOM | 1636 1637 | | GLU GLU | 206 | | 14.487 | 17.502 | | _ | 0 27.89 | AAAA |
| MOTA MOTA | 1638 | | GLU | 206 | | 13.345 | 16.816 | | | 0 28.90 | AAAA AAAA |
| MOTA | 1639 | | | 206 | | 12.060 | 17.615 | | | 00 48.55 | AAAA |
| MOTA | 1640 | | | 206 | | 12.169 | 18.832 | | _ | 0 21.58 | AAAA |
| MOTA | 1641 | OE | 1 GLU | 206 | | 11.360 | | | _ | 0 63.58 | AAAA |
| MOTA | 1642 | | 2 GLU | 206 | | 13.076 | | | _ | 00 22.86 | AAAA |
| MOTA | 1643 | | GLU | 206 | | 15.819 | | - | | 00 21.21 | AAAA |
| MOTA | 1644 | | GLU | 206 | | 16.071 16.666 | | | 1.0 | 00 25.04 | AAAA |
| ATOM | 1645 | | GLU | 207 | | 17.976 | | | 2 1.0 | 00 19.61 | AAAA |
| ATOM | 1646 | | | 207 207 | | 18.483 | | | 1.0 | 00 20.75 | AAAA |
| ATOM | | | | 207 | | 17.682 | 18.22 | 2 56.753 | 3 1.0 | 00 18.44 | AAAA AAAA |
| MOTA | | | | 207 | | 17.687 | 19.51 | 4 55.983 | | 00 24.75 | AAAA AAAA |
| MOTA MOTA | | | 1 GLU | 207 | | 18.738 | | 2 55.948 | 3 1. | 00 22.17 | , |
| ATOM | | | | • | | | | = | | | |
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|--------------|--------------|---------|------------|------------|------------|--------------|------------------------|------------------|--------|----------------|--------------|
| | | 022 | GLU | 207 | 16.6 | 346 | 19.854 | 55.396 | 1.00 | | AAAA |
| MOTA | 1651 | | GFO | 207 | 18.9 | | 17.379 | 60.350 | 1.00 2 | | AAAA |
| ATOM | 1652 1653 | 0 | GLU | 207 | 19.5 | | 18.416 | 60.687 | 1.00 | | AAAA |
| ATOM | 1654 | N | ILE | 208 | 19.0 | | 16.218 | 60.988 | 1.00 | | AAAA AAAA |
| ATOM ATOM | 1655 | CA | ILE | 208 | 19.9 | | 16.138 | 62.168 | 1.00 | | AAAA |
| ATOM | 1656 | СВ | ILE | 208 | 19.1 | | 15.652 | 63.403 | 1.00 | | AAAA |
| ATOM | 1657 | CG2 | ILE | 208 | 19.9 | | 15.693 | 64.653 | 1.00 | 11 61 | AAAA |
| ATOM | 1658 | CG1 | | 208 | 17.9 | | 16.561 | 63.625 64.786 | 1.00 | | AAAA |
| ATOM | 1659 | CD1 | ILE | .208 | 17.0 | | 16.160 15.260 | 61.981 | 1.00 | | AAAA |
| MOTA | 1660 | C | ILE | 208 | 21. | | 14.850 | 62.943 | 1.00 | | AAAA |
| ATOM | 1661 | 0 | ILE | 208 | 21. 21. | | 14.850 | 60.738 | 1.00 | | AAAA |
| MOTA | 1662 | N | GLY | 209 | 22. | | 14.153 | 60.535 | 1.00 | 20.43 | AAAA |
| MOTA | 1663 | CA | GLY | 209 209 | 22. | | 12.769 | 60.037 | 1.00 | 25.56 | AAAA |
| MOTA | 1664 | C | GLY GLY | 209 | 21. | | 12.447 | 59.850 | 1.00 | 25.22 | AAAA |
| MOTA | 1665 | N | GLU | 210 | 23. | | 11.944 | 59.888 | 1.00 | 26.07 | AAAA |
| MOTA | 1666 1667 | CA | GLU | 210 | 23. | | 10.601 | 59.348 | 1.00 | 25.78 | AAAA AAAA |
| MOTA | 1668 | CB | GLU | 210 | 23. | 404 | 10.731 | 57.835 | 1.00 | 28.27 | AAAA |
| MOTA MOTA | 1669 | CG | GLU | 210 | 23. | | 9.569 | 56.965 | 1.00 | 56.41 65.37 | AAAA |
| ATOM | 1670 | CD | GLÜ | 210 | 23. | | 9.952 | 55.495 55.075 | 1.00 | 62.00 | AAAA |
| | - 1671 | OE1 | GLU | 210 | 24. | | 10.327 | 54.768 | 1.00 | 73.24 | AAAA |
| ATOM | 1672 | OE2 | GLU | 210 | 22. | | 9.89 4 9.709 | 59.936 | 1.00 | 31.85 | AAAA |
| ATOM | 1673 | С | GLU | 210 | 24. 25. | | 10.170 | 60.217 | 1.00 | 28.85 | AAAA |
| MOTA | 1674 | 0 | GLU | 210 | | 012 | 8.431 | 60.121 | 1.00 | 27.84 | AAAA |
| ATOM | 1675 | N | GLY | 211 211 | | 991 | 7.502 | 60.657 | 1.00 | 26.25 | AAAA |
| ATOM | 1676 | CA | GLY GLY | 211 | | 545 | 7.942 | 61.995 | 1.00 | 27.79 | AAAA |
| ATOM | 1677 1678 | С 0 | GLY | 211 | | 788 | 8.324 | 62.874 | 1.00 | 28.66 | AAAA |
| ATOM | 1679 | Ŋ | LYS | 212 | 26. | 865 | 7.880 | 62.150 | 1.00 | 34.62 | aaaa aaaa |
| MOTA MOTA | 1680 | CA | LYS | 212 | | 512 | 8.287 | 63.393 | 1.00 | 34.39 40.40 | AAAA |
| ATOM | 1681 | CB | LYS | 212 | | 029 | 8.132 | 63.273 | 1.00 | 53.97 | AAAA |
| ATOM | 1682 | CG | LYS | 212 | | 505 | 6.712 | 62.996 | 1.00 | 61.93 | AAAA |
| ATOM | 1683 | CD | LYS | 212 | | 139 | 5.770 | 64.131 63.863 | 1.00 | 62.74 | AAAA |
| ATOM | 1684 | CE | LYS | 212 | | 612 | 4.347 4.258 | 63.711 | 1.00 | 70.11 | AAAA |
| ATOM | 1685 | NZ | LYS | 212 | | 091 181 | 9.741 | 63.725 | 1.00 | 36.04 | AAAA |
| ATOM | 1686 | C | LYS | 212 | | 109 | 10.126 | 64.897 | 1.00 | 28.34 | AAAA |
| MOTA | 1687 | 0 | LYS | 212 213 | _ | 959 | 10.543 | 62.688 | 1.00 | 31.47 | AAAA |
| MOTA | 1688 | N CA | GLY GLY | 213 | | 648 | 11.948 | 62.898 | 1.00 | 31.68 | AAAA |
| MOTA | 1689 1690 | CA | GLY | 213 | | .189 | 12.291 | 63.142 | 1.00 | 28.78 | аааа аааа |
| MOTA | 1691 | 0 | GLY | 213 | 24 | .840 | 13.460 | 63.259 | 1.00 | 22.56 | AAAA |
| MOTA MOTA | 1692 | N | LYS | 214 | | .317 | 11.292 | 63.222 | 1.00 | 28.54 31.11 | AAAA |
| ATOM | 1693 | CA | LYS | 214 | | .905 | 11.585 | 63.463 63.325 | 1 00 | 31.03 | AAAA |
| ATOM | 1694 | CB | LYS | 214 | | .080 | 10.295 10.461 | 63.224 | 1 00 | 38.15 | AAAA |
| ATOM | 1695 | CG | | 214 | | .583 | 9.115 | 62.844 | 1.00 | 40.49 | AAAA |
| MOTA | 1696 | CD | _ | 214 | | .968 .490 | 9.220 | | 1.00 | 48.02 | AAAA |
| ATOM | 1697 | CE | | 214 | | .927 | 7.924 | | 1.00 | 44.99 | AAAA |
| ATOM | 1698 | NZ | | 214 214 | | .834 | 12.160 | | 1.00 | 26.90 | AAAA |
| ATOM | 1699 | C | LYS LYS | 214 | 23 | .260 | 11.524 | 65.831 | | 33.33 | AAAA |
| MOTA | 1700 | O N | GLY | 215 | | .310 | 13.376 | | | 24.38 | AAAA AAAA |
| MOTA | 1701 1702 | CA | | 215 | 22 | .230 | 14.034 | | | 26.03 | AAAA |
| MOTA | 1702 | C | GLY | 215 | 23 | .298 | 15.115 | | | 27.03 | AAAA |
| MOTA MOTA | 1703 | | GLY | 215 | 23 | .352 | 15.820 | | | 23.34 | AAAA |
| ATOM | 1705 | | TYR | 216 | | .152 | 15.260 | | | 25.51 | AAAA |
| ATOM | 1706 | | | 216 | | .217 | | | | 20.54 | AAAA |
| ATOM | 1707 | | TYR | 216 | 26 | .592 | 15.576 | | | 26.47 | AAAA |
| ATOM | 1708 | CG | | 216 | 26 | .900 | 14.671 13.464 | | | 28.96 | AAAA |
| ATOM | 1709 | | 1 TYR | 216 | | .221 | | | 1.00 | 33.08 | AAAA |
| ATOM | 1710 | | | 216 | | .455 .832 | | | 1.0 | 24.21 | AAAA |
| ATOM | 1711 | | | 216 | 21 | .074 | 14.254 | | 1.0 | 34.45 | AAAA |
| ATOM | | | | 216 | | .378 | | | 1.0 | 0 40.53 | AAAA |
| ATOM | | | | 216 216 | | .580 | | | 1.0 | 0 45.67 | AAAA |
| ATOM | | | | | | .104 | 17.39 | 64.493 | | 0 22.57 | AAAA |
| ATOM | | | TYR | | | .097 | | 4 64.12 | 5 1.0 | 0 19.70 | AAAA |
| ATOM | | , . | | | | | | - | | | • |
| • | | | | | | | | | | | |

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|--------------|--------------|------------|------------|------------|------------------|------------------|-------------------|--------------------------|--------------|
| | | | ASN | 217 | 23.889 | 17.635 | | 1.00 22.88 | AAAA |
| MOTA | 1717 1718 | | asn Asn | 217 | 23.621 | 18.729 | | 1.00 22.60 | AAAA AAAA |
| MOTA | 1719 | | ASN | 217 | 23.453 | 18.240 | | 1.00 16.61 | AAAA |
| MOTA MOTA | 1720 | | ASN | 217 | 23.233 | 19.387 | — - · · · | 1.00 17.16 1.00 20.23 | AAAA |
| ATOM | 1721 | OD1 | ASN | 217 | 22.098 | 19.704 | 60.307 60.309 | 1.00 20.23 | AAAA |
| MOTA | 1722 | ND2 | | 217 | 24.320 | 20:032 | 63.630 | 1.00 17.65 | AAAA |
| MOTA | 1723. | С | asn | 217 | 22.311 | 19.296 18.550 | 63.894 | 1.00 17.63 | AAAA |
| ATOM | 1724 | _ | ASN | 217 | 21.381 22.236 | 20.610 | 63.793 | 1.00 21.68 | AAAA |
| MOTA | 1725 | | LEU | 218 | 21.014 | 21.197 | 64.320 | 1.00 21.20 | AAAA |
| MOTA | 1726 | | LEU | 218 218 | 21.186 | 21.547 | 65.808 | 1.00 17.73 | AAAA |
| MOTA | 1727 | | LEU LEU | 218 | 19.906 | 21.702 | 66.647 | 1.00 32.30 | AAAA |
| MOTA | 1728 1729 | CG CD1 | | 218 | 20.228 | 22.427 | 67.944 | 1.00 24.51 | AAAA AAAA |
| ATOM ATOM | 1730 | CD2 | | 218 | 18.862 | 22.464 | 65.903 | 1.00 40.08 1.00 19.46 | AAAA |
| MOTA | 1731 | c | LEU | 218 | 20.700 | 22.459 | 63.554 63.615- | 1.00 19.40 | AAAA |
| ATOM | 1732 | Ō | LEU | 218 | 21.467 | 23.425 | 62.824 | 1.00 15.43 | AAAA |
| ATOM | 1733 | N | ASN | 219 | 19.590 | 22.441 23.609 | 62.072 | 1.00 14.05 | AAAA |
| MOTA | 1734 | CA | ASN | 219 | 19.143 18.634 | 23.232 | 60.665 | 1.00 15.92 | AAAA |
| MOTA | 1735 | CB | ASN | 219 | 19.732 | 22.738 | 59.750 | 1.00 22.73 | AAAA |
| MOTA | 1736 | CG OD1 | ASN | 219 219 | 20.861 | 23.232 | 59.802 | 1.00 17.90 | AAAA |
| ATOM | 1737 | ND2 | | 219 | 19.398 | 21.789 | 58.868 | 1.00 16.62 | AAAA |
| MOTA | 1738 1739 | C | ASN | 219 | 17.990 | 24.256 | 62.821 | 1.00 21.98 | AAAA AAAA |
| MOTA | 1740 | Õ | ASN | 219 | 17.075 | 23.569 | 63.262 | 1.00 18.65 1.00 16.82 | AAAA |
| MOTA MOTA | 1741 | N | ILE | 220 | 18.025 | 25.580 | 62.952 63.640 | 1.00 13.32 | AAAA |
| ATOM | 1742 | CA | ILE | 220 | 16.951 | 26.298 27.115 | 64.823 | 1.00 15.70 | AAAA |
| ATOM | 1743 | CB | ILE | 220 | 17.522 | 27.113 | 65.479 | 1.00 15.18 | AAAA |
| MOTA | 1744 | CG2 | ILE | 220 | 16.411 18.246 | 26.193 | 65.823 | 1.00 19.11 | AAAA |
| ATOM | 1745 | | ILE ILE | 220 220 | 17.350 | 25.259 | 66.632 | 1.00 22.75 | AAAA |
| MOTA | 1746 | CDI | ILE | 220 | 16.363 | 27.246 | 62.573 | 1.00 18.80 | AAAA |
| MOTA | 1747 1748 | 0 | ILE | 220 | 16.810 | 28.386 | 62.419 | 1.00 15.52 | AAAA AAAA |
| MOTA MOTA | 1749 | N | PRO | 221 | 15.341 | 26.790 | 61.826 | 1.00 16.72 1.00 18.83 | AAAA |
| ATOM | 1750 | CD | PRO | | 14.612 | 25.518 | 61.906 60.785 | 1.00 10.03 | AAAA |
| MOTA | 1751 | CA | PRO | 221 | 14.739 | 27.628 26.615 | 59.948 | 1.00 20.76 | AAAA |
| ATOM | 1752 | CB | PRO | 221 | 13.930 14.409 | 25.241 | 60.462 | 1.00 28.73 | AAAA |
| MOTA | 1753 | CG | PRO | 221 | 13.849 | 28.664 | 61.444 | 1.00 21.26 | AAAA |
| MOTA | 1754 | C | PRO | 221 221 | 13.061 | 28.318 | 62.314 | 1.00 22.46 | AAAA |
| ATOM | 1755 | O N | PRO LEU | 222 | 13.977 | 29.926 | 61.028 | 1.00 19.70 | AAAA AAAA |
| MOTA | 1756 1757 | CA | LEU | 222 | 13.209 | 31.018 | | 1.00 21.62 1.00 16.46 | AAAA |
| MOTA MOTA | 1758 | CB | LEU | 222 | 14.163 | 31.972 | | 1.00 18.65 | AAAA |
| MOTA | 1759 | CG | LEU | 222 | 14.868 | | | | AAAA |
| ATOM | 1760 | | LEU | 222 | 16.026 13.857 | | | 1.00 19.98 | AAAA |
| MOTA | 1761 | | LEU | 222 | 12.350 | | 60 500 | 1.00 19.68 | AAAA |
| MOTA | 1762 | | LEU | 222 222 | 12.687 | 31.830 | | 1.00 18.07 | AAAA |
| ATOM | 1763 | | LEU PRO | 223 | 11.220 | 32.329 | 61.042 | | AAAA AAAA |
| ATOM | 1764 1765 | | PRO | 223 | 10.723 | 32.249 | | | AAAA |
| MOTA MOTA | 1766 | | PRO | 223 | 10.264 | | | | AAAA |
| ATOM | 1767 | | PRO | 223 | 9.006 | | | | AAAA |
| MOTA | 1768 | | PRO | 223 | 9.608 | | | | AAAA |
| ATOM | 1769 | | PRO | 223 | 10.606 | | | | AAAA |
| MOTA | 1770 | | PRO | 223 | 11.525 9.830 | | | 1.00 16.41 | AAAA |
| ATOM | | | LYS | 224 224 | 9.975 | | | 1.00 16.11 | AAAA |
| ATOM | | | | 224 | 9.002 | | 57.039 | | AAAA |
| MOTA | | | | 224 | 9.163 | 35.44 | | | AAAA AAAA |
| ATOM | | | | 224 | 8.109 | 35.68 | | | AAAA |
| MOTA MOTA | | • | | 224 | 8.209 | 34.62 | | | AAAA |
| ATOM | | | | 224 | | 7 34.84 | | | AAAA |
| ATOM | | | LYS | 224 | 9.631 8.81 | | | 6 1.00 21.07 | AAAA |
| ATOM | 177 | 9 0 | LYS | 224 | 10.23 | | 9 59.17 | 1 1:00 20.77 | AAAA |
| ATOM | 178 | | GLY | | 9.97 | | 7 60.12 | 9 1.00 20.30 | AAAA |
| ATOM | | | GLY GLY | | 10.55 | | | | AAAA |
| MOTA | 178 | د <i>د</i> | | | | | - | | |

| . =01/ | 1702 | ^ | GLY | 225 | 10 | 128 | 39.912 | | 1.00 20. | 66 AAAA | |
|--------------|--------------|-----------|---------|------|-----|--------|---------|----------|--------------------|---------------------------------------|--|
| ATOM | 1783 | - | LEU | 226 | 11 | 1.540 | 38.395 | 61.606 | 1.00 20. | 37 AAAA | |
| MOTA | 1784 | | LEU | 226 | 12 | 2.154 | 38.063 | 62.893 | 1.00 18. | | |
| ATOM | 1785 | | LEU | 226 | 1. | 3.354 | 37.145 | 62.670 | 1.00 13. | 63 AAAA | |
| ATOM | 1786 1787 | | LEU | 226 | 13 | 3.836 | 36.443 | 63.939 | 1.00 18. | | |
| MOTA | _ | CD1 | | 226 | 12 | 2.834 | 35.329 | 64.243 | 1.00 18. | | |
| ATOM - | 1788 | CD2 | | 226 | | 5.232 | 35.844 | 63.741 | 1.00 17. | | |
| ATOM | 1789 | | LEU | 226 | | 2.649 | 39.309 | 63.642 | 1.00 19. | | |
| MOTA | 1790 | | LEU | 226 | | 3.320 | 40.151 | 63.052 | 1.00 18. | | |
| MOTA | 1791 | - | ASN | 227 | | 2.336 | 39.421 | 64.932 | 1.00 23. | | |
| ATOM | 1792 | N | ASN | 227 | | 2.815 | 40.571 | 65.692 | 1.00 20. | | |
| MOTA | 1793 | | ASN | .227 | | 1.682 | 41.261 | 66.485 | 1.00 21. | 73 AAAA | |
| MOTA | 1794 | CB | ASN | 227 | | 1.061 | 40.368 | 67.546 | 1.00 20. | | |
| MOTA | 1795 | CG OD1 | | 227 | | 1.762 | 39.736 | 68.341 | 1.00 23. | | |
| MOTA | 1796 | ND2 | | 227 | _ | 9.729 | 40.340 | 67.581 | 1.00 21. | | |
| MOTA | 1797 | | ASN | 227 | | 3.950 | 40.152 | 66.612 | 1.00 25. | 24 -AAAA | |
| MOTA | 1798 | C | asn | 227 | | 4.282 | 38.965 | 66.702 | 1.00 18. | 54 AAAA | |
| MOTA | 1799 | 0 | ASP | 228 | _ | 4.547 | 41.124 | 67.296 | 1.00 19. | 41 AAAA | |
| MOTA | 1800 | N | ASP | 228 | | 5.682 | 40.844 | 68.169 | 1.00 22. | | |
| MOTA | 1801 | CA | ASP | 228 | _ | 6.208 | 42.141 | 68.802 | 1.00 16. | | |
| MOTA | 1802 | CB CG | ASP | 228 | | 6.852 | 43.060 | 67.796 | 1.00 30. | 68 AAAA | |
| ATOM | 1803 | OD1 | | 228 | | 7.182 | 42.576 | 66.690 | 1.00 23 | .87 AAAA | |
| ATOM | 1804 | | ASP | 228 | 1 | 7.053 | 44.256 | 68.123 | 1.00 25 | | |
| ATOM | 1805 | C | ASP | 228 | 1 | 5.440 | 39.835 | 69.265 | 1.00 18 | | |
| MOTA | 1806 | 0 | ASP | 228 | 1 | 6.298 | 39.002 | 69.536 | 1.00 16 | | |
| MOTA | 1807 1808 | N | ASN | 229 | 1 | 4.291 | 39.930 | 69.928 | 1.00 20 | | |
| MOTA | 1809 | CA | ASN | 229 | 1 | 3.975 | 39.015 | 71.007 | 1.00 21 | .75 AAAA .46 AAAA | |
| ATOM | 1810 | CB | ASN | 229 | 1 | 2.706 | 39.483 | 71.712 | 1.00 19 | | |
| ATOM | 1811 | CG | ASN | 229 | | 2.943 | 40.738 | 72.516 | 1.00 27 | · - - | |
| MOTA | 1812 | | ASN | 229 | 1 | 3.588 | 40.691 | 73.556 | 1.00 33 | | |
| ATOM | 1813 | | ASN | 229 | · 1 | 2.464 | 41.874 | 72.019 | 1.00 21 | | |
| MOTA | 1814 | C | ASN | 229 | | 13.833 | 37.596 | 70.503 | 1.00 18 | | |
| MOTA | 1815 | Ö | ASN | 229 | 1 | L4.284 | 36.644 | 71.151 | 1.00 22 | • - : | |
| ATOM | 1816 | Ŋ | GLU | 230 | | 13.252 | 37.454 | 69.319 | 1.00 17 | • - | |
| MOTA | 1817 | CA | GLU | 230 | 1 | 13.081 | 36.125 | 68.748 | 1.00 21 | | |
| ATOM | 1818 | CB | GLU | 230 | - | 12.152 | 36.193 | 67.536 | 1.00 20 | | |
| MOTA | 1819 | CG | GLU | 230 | : | 10.765 | 36.714 | 67.890 | 1.00 28 | | |
| MOTA | 1820 | CD | GLU | 230 | | 9.870 | 36.816 | 66.677 | 1.00 24 | | |
| MOTA MOTA | 1821 | | GLU | 230 | : | 10.360 | | | 1.00 22 1.00 24 | | |
| ATOM | 1822 | | GLU | 230 | | 8.683 | 36.443 | | 1.00 24 | | |
| ATOM | 1823 | c | GLU | 230 | | 14.422 | | | 1.00 10 | · · · · · · · · · · · · · · · · · · · | |
| MOTA | 1824 | ō | GLU | 230. | | 14.663 | 34.326 | | 1.00 15 | , | |
| MOTA | 1825 | N | PHE | 231 | | 15.305 | | | 1.00 15 | | |
| ATOM | 1826 | CA | PHE | 231 | | 16.616 | | | 1.00 13 | | |
| ATOM | 1827 | CB | PHE | 231 | | 17.420 | | | | | |
| ATOM | 1828 | CG | PHE | 231 | | 18.719 | 36.361 | 66.069 | | | |
| ATOM | 1829 | | PHE | 231 | | 18.723 | 35.445 | 65.016 | | | |
| ATOM | 1830 | | PHE | 231 | | 19.936 | | | | | |
| ATOM | 1831 | | PHE | 231 | | 19.918 | | | | | |
| ATOM | 1832 | | PHE | 231 | | 21.144 | | | | | |
| MOTA | 1833 | CZ | PHE | 231 | | 21.130 | 35.431 | | | | |
| ATOM | 1834 | С | PHE | 231 | | 17.385 | | | | | |
| MOTA | 1835 | 0 | PHE | 231 | | 17.869 | | | | ,,,,, | |
| MOTA | 1836 | N | LEU | 232 | | 17.495 | | | | | |
| MOTA | 1837 | CA | LEU | 232 | | 18.239 | 35.850 | | | | |
| ATOM | 1838 | | LEU | 232 | | 18.41 | | | | -, | |
| ATOM | 1839 | | LEU | 232 | | 19.214 | | | | | |
| ATOM | 1840 | | 1 LEU | 232 | | 19.13 | | | | | |
| ATOM | 1841 | | 2 LEU | 232 | | 20.65 | | | | • • • • | |
| ATOM | 1842 | | LEU | 232 | | 17.60 | | | | | |
| ATOM | 1843 | | LEU | 232 | | 18.30 | | | | | |
| ATOM | 1844 | | PHE | 233 | | 16.28 | | | | | |
| MOTA | 1845 | | | 233 | | 15.58 | 7 33.53 | | | | |
| ATOM | 1846 | | | | | 14.07 | | 3 72.095 | | | |
| ATOM | | | | | | 13.28 | | | | * | |
| ATOM | | | 1 PHE | | | 12.86 | 3 32.30 | 2 73.84 | 1 1.00 2 | | |
| MOTA | | | · · · · | ٠. | • | | | | | | |

| | | | | | | 22 477 | 71.596 | 1.00 19.92 | AAAA |
|------|-------|-----|---------|-----|---------|-----------|----------|--------------|------|
| ATOM | 1849 | CD2 | PHE | 233 | 12.942 | 31.473 | | 1.00 29.35 | AAAA |
| | 1850 | CE1 | PHE | 233 | 12.088 | 31.206 | | 1.00 25.33 | AAAA |
| MOTA | 1851 | | PHE | 233 | 12.168 | 30.363 | | 1.00 25.37 | AAAA |
| MOTA | | | PHE | 233 | 11.737 | 30.231 | | 1.00 30.28 | |
| ATOM | 1852 | CZ | | 233 | 16.041 | 32.234 | 71.660 | 1.00 23.12 | AAAA |
| ATOM | 1853 | С | PHE | | 16.433 | 31.273 | 72.332 | 1.00 18.35 | AAAA |
| ATOM | 1854 | 0 | PHE | 233 | | 32.208 | 70.332 | 1.00 17.26 | AAAA |
| ATOM | 1855 | N | ALA | 234 | 15.961 | | 69.562 | 1.00 17.67 | AAAA |
| ATOM | 1856 | CA | ALA | 234 | 16.332 | | 68.046 | 1.00 19.08 | AAAA |
| | 1857 | CB | ALA | 234 | 16.085 | | 68.040 | 1.00 15.00 | AAAA |
| ATOM | 1858 | C | ALA | 234 | 17.786 | | 69.800 | 1.00 16.31 | AAAA |
| ATCM | | 0 | ALA | 234 | 18.127 | 29.461 | 69.926 | 1.00 16.75 | |
| MOTA | 1859 | | | 235 | 18.646 | 31.643 | 69.846 | 1.00 16.73 | AAAA |
| ATOM | 1860 | N | LEU | 235 | 20.074 | 31.411 | 70.051 | 1.00 19.14 | AAAA |
| MOTA | 1861 | CA | LEU | | 20.823 | | 69.956 | 1.00 21.72 | AAAA |
| ATOM | 1862 | CB | LEU | 235 | | | 69.345 | 1.00 36.73 | AAAA |
| ATOM | 1863 | CG | LEU | 235 | 22.226 | | 70.105 | 1.00 20.69 | AAAA |
| MOTA | 1864 | CD1 | LEU | 235 | 23.026 | | 69.393 | 1.00 22.96 | AAAA |
| ATOM | 1865 | CD2 | LEU | 235 | 22.917 | | | 1.00 18.71 | AAAA |
| | 1866 | C | LEU | 235 | 20.354 | | 71.421 | 1.00 18.72 | AAAA |
| ATOM | 1867 | Ö | LEU | 235 | 21.028 | | 71.522 | 1.00 10.33 | AAAA |
| MOTA | | | GLU | 236 | 19.83 | 31.390 | 72.479 | 1.00 25.43 | |
| MOTA | 1868 | N | | 236 | 20.04 | | 73.839 | 1.00 19.75 | AAAA |
| MOTA | 1869 | CA | GLU | | 19.33 | | 74.860 | 1.00 23.18 | AAAA |
| ATOM | 1870 | CB | GLU | 236 | | | 74.777 | 1.00 38.53 | AAAA |
| ATOM | 1871 | CG | GLU | 236 | 19.72 | | 75.648 | 1.00 42.42 | AAAA |
| MOTA | 1872 | CD | GLU | 236 | 18:85 | | 75.428 | 1.00 45.43 | AAAA |
| ATOM | 1873 | OE1 | GLU | 236 | 17.61 | | | 1.00 48.76 | AAAA |
| | 1874 | | GLU | 236 | 19.42 | | 76.548 | 1.00 25.85 | AAAA |
| MOTA | | C | GLU | 236 | 19.54 | 1 29.452 | 74.011 | 1.00 25.65 | AAAA |
| ATOM | 1875 | | GLU | 236 | 20.22 | | 74.597 | 1.00 21.36 | AAAA |
| MOTA | 1876 | 0 | | 237 | 18.34 | 3 29.193 | 73.501 | 1.00 23.16 | |
| ATOM | 1877 | N | LYS | | 17.75 | | 73.610 | 1.00 17.06 | AAAA |
| MOTA | 1878 | CA | LYS | 237 | 16.28 | | 73.193 | 1.00 26.98 | AAAA |
| ATOM | 1879 | CB | LYS | 237 | 15.48 | | | 1.00 52.00 | AAAA |
| MOTA | 1880 | CG | LYS | 237 | _ | | | 1.00 56.40 | AAAA |
| ATOM | 1881 | CD | LYS | 237 | 14.07 | - | | 1.00 52.03 | AAAA |
| ATOM | 1882 | CE | LYS | 237 | 14.13 | | | 1.00 55.53 | AAAA |
| | 1883 | NZ | LYS | 237 | 12.78 | | | 1.00 18.46 | AAAA |
| MOTA | 1884 | C | LYS | 237 | 18.50 | | | 1.00 10.40 | AAAA |
| MOTA | | | LYS | 237 | 18.69 | 1 25.692 | 73.231 | 1.00 21.20 | AAAA |
| MOTA | 1885 | 0 | | 238 | 18.93 | | 71.578 | 1.00 21.28 | |
| MOTA | 1886 | N | SER | | 19.64 | | 70.776 | 1.00 16.47 | AAAA |
| ATOM | 1887 | CA | SER | 238 | 19.74 | | | 1.00 19.75 | AAAA |
| ATOM | 1888 | CB | SER | 238 | 20.47 | - | | 1.00 22.52 | АААА |
| ATOM | 1889 | OG | SER | 238 | | | | 1.00 18.79 | AAAA |
| MOTA | 1890 | С | SER | 238 | 21.03 | | | 1.00 20.60 | AAAA |
| ATOM | 1891 | 0 | SER | 238 | 21.52 | | | 1.00 22.95 | AAAA |
| MOTA | 1892 | N | LEU | 239 | 21.69 | 0 26.937 | | 1.00 20.98 | AAAA |
| | 1893 | CA | LEU | 239 | 23.00 | 26.701 | | 1.00 18.39 | AAAA |
| MOTA | | CB | | 239 | 23.6 | 28.008 | | 1.00 10.33 | AAAA |
| MOTA | 1894 | | | 239 | 23.9 | 35 29.072 | 2 71.933 | 1.00 20.02 | AAAA |
| MOTA | 1895 | CG | - 1 FII | 239 | 24.5 | 38 30.31 | 1 72.636 | | |
| ATOM | 1896 | | 1 LEU | | 25.0 | | 6 70.933 | 1.00 20.31 | AAAA |
| ATOM | 1897 | CD | 2 LEU | 239 | 22.8 | | | 1.00 25.16 | AAAA |
| MOTA | 1898 | С | LEU | 239 | | | | | AAAA |
| ATOM | 1899 | 0 | LEU | 239 | 23.7 | | | | AAAA |
| ATOM | | | GLU | 240 | 21.7 | | · | | AAAA |
| | | | GLU | 240 | 21.5 | | | | AAAA |
| ATOM | | | | 240 | 20.3 | 31 25.35 | | | AAAA |
| ATOM | | | | 240 | 20.0 | 42 24.53 | | | AAAA |
| MOTA | | | | 240 | 19.0 | 53 25.21 | 2 78.515 | | |
| MOTA | 1904 | | | | 17.9 | | 0 78.067 | | AAAA |
| MOTA | 1905 | | E1 GLU | 240 | 10 4 | | | 1.00 66.68 | AAAA |
| ATOM | | | | | 19.4 | | | 1.00 23.44 | AAAA |
| ATOM | | 7 C | GLU | 240 | 21.4 | | | | AAAA |
| ATOM | | | GLU | 240 | 21.9 | | | | AAAA |
| | | | | 241 | 20.7 | | | | AAAA |
| ATOM | | | | | 20.5 | | | | AAAA |
| ATOM | | - | | | 19.7 | 05 22.03 | 9 72.05 | | AAAA |
| ATOM | 191 | | | | 19.7 | | 8 71.32 | | |
| ATOM | | | 32 ILE | | 18.2 | | | 1.00 28.60 | AAAA |
| ATOM | 1 191 | | G1 ILE | | 17.3 | | | 7 1.00 27.04 | AAAA |
| ATOM | | 4 C | D1 ILE | 241 | £ / • = | | • | • | • |
| | | | | • | • | | | | |

| | | | | | 21.957 | 21.404 | 72.941 | 1.00 25.48 | AAAA |
|------|------|--------|------------|-----|------------------|--------|--------|-------------|-------|
| MOTA | 1915 | C | ILE | 241 | 22.244 | 20.234 | 73.195 | 1.00 19.43 | AAAA |
| MOTA | 1916 | 0 | ILE | 241 | 22.799 | 22.235 | 72.334 | 1.00 20.41 | AAAA |
| ATOM | 1917 | | VAL | 242 | | 21.782 | 71.928 | 1.00 23.17 | AAAA |
| MOTA | 1918 | | VAL | 242 | 24.116 24.853 | 22.856 | 71.107 | 1.00 26.48 | AAAA |
| ATOM | 1919 | | VAL | 242 | | | 70.807 | 1.00 18.67 | AAAA |
| ATOM | 1920 | CG1 | | 242 | 26.273 | 22.394 | 69.802 | 1.00 26.97 | AAAA |
| ATOM | 1921 | CG2 | VAL | 242 | 24.093 | 23.135 | | 1.00 24.81 | AAAA |
| ATOM | 1922 | С | VAL | 242 | 24.962 | 21.456 | 73.154 | 1.00 22.49 | AAAA |
| ATOM | 1923 | 0 | VAL | 242 | 25.566 | 20.384 | 73.235 | 1.00 25.06 | AAAA |
| ATOM | 1924 | N | LYS | 243 | 24.989 | 22.387 | 74.102 | 1.00 25.00 | AAAA |
| ATOM | 1925 | CA | LYS | 243 | 25.775 | 22.202 | 75.311 | | AAAA |
| ATOM | 1926 | CB | LYS | 243 | 25.599 | 23.379 | 76.272 | 1.00 28.53 | AAAA |
| ATOM | 1927 | CG | LYS | 243 | 26.386 | 23.183 | 77.568 | 1.00 43.21 | AAAA |
| ATOM | 1928 | CD | LYS | 243 | 26.022 | 24.191 | 78.653 | 1.00 53.10 | AAAA |
| MOTA | 1929 | CE | LYS | 243 | 26.407 | 25.607 | 78.287 | 1.00 50.30 | AAAA |
| MOTA | 1930 | NZ | LYS | 243 | 26.045 | 26.548 | 79.389 | 1.00 59.15 | |
| ATOM | 1931 | C | LYS | 243 | 25.433 | 20.917 | 76.046 | 1.00 30.38 | AAAA |
| ATOM | 1932 | Õ | LYS | 243 | 26.321 | 20.255 | 76.578 | 1.00 35.44 | AAAA |
| | 1933 | N | GLU | 244 | 24.161 | 20.542 | 76.076 | 1.00 28.12 | AAAA |
| MOTA | 1934 | CA | GLU | 244 | 23.798 | 19.320 | 76.798 | 1.00 37.54 | AAAA |
| ATOM | 1935 | CB | GLU | 244 | 22.288 | 19.260 | 77.048 | 1.00 35.34 | AAAA |
| MOTA | 1936 | CG | GLU | 244 | 21.735 | 20.459 | 77.816 | 1.00 55.88 | AAAA |
| ATOM | 1937 | CD | GLU | 244 | 20.281 | 20.275 | 78.230 | 1.00 57.89 | AAAA |
| MOTA | 1938 | - | GLU | 244 | 19.673 | 21.246 | 78.738 | 1.00 60.60 | AAAA |
| ATOM | 1939 | | GLU | 244 | 19.753 | 19.152 | 78.062 | 1.00 57.73 | AAAA |
| ATOM | | C | GLU | 244 | 24.231 | 18.034 | 76.102 | 1.00 38.17 | AAAA |
| MOTA | 1940 | | GLU | 244 | 24.294 | 16.978 | 76.727 | 1.00 38.46 | AAAA |
| ATOM | 1941 | N O | VAL | 245 | . 24.541 | 18.124 | 74.817 | 1.00 30.29 | AAAA |
| ATOM | 1942 | | VAL | 245 | 24.933 | 16.958 | 74.042 | 1.00 29.17 | AAAA |
| ATOM | 1943 | CA | VAL | 245 | 23.984 | 16.778 | 72.833 | 1.00 46.68 | AAAA |
| MOTA | 1944 | CB | VAL | 245 | 24.462 | 15.641 | 71.942 | 1.00 53.09 | AAAA |
| ATOM | 1945 | | VAL | 245 | 22.581 | 16.488 | 73.327 | 1.00 54.19 | AAAA |
| MOTA | 1946 | | VAL | 245 | 26.364 | 16.982 | 73.508 | 1.00 34.90 | AAAA |
| ATOM | 1947 | C | VAL | 245 | 26.915 | 15.939 | 73.164 | 1.00 34.73 | AAAA |
| MOTA | 1948 | 0 | PHE | 246 | 26.980 | 18.156 | 73.465 | 1.00 29.22 | AAAA |
| MOTA | 1949 | N | | 246 | 28.324 | 18.256 | 72.897 | 1.00 29.17 | AAAA |
| MOTA | 1950 | CA | PHE PHE | 246 | 28.178 | 18.800 | 71.464 | 1:00 30.42 | AAAA |
| MOTA | 1951 | CB | PHE | 246 | 29.384 | 18.588 | 70.585 | 1.00 25.62 | AAAA |
| MOTA | 1952 | CG | PHE | 246 | 29.695 | 17.326 | 70.097 | 1.00 28.89 | AAAA |
| ATOM | 1953 | | PHE | 246 | 30.167 | 19.668 | 70.196 | 1.00 25.17 | AAAA |
| ATOM | 1954 | | | 246 | 30.771 | 17.138 | 69.222 | 1.00 23.43 | AAAA |
| ATOM | 1955 | | PHE | 246 | 31.248 | 19.495 | 69.322 | 1.00 22.40 | AAAA |
| ATOM | 1956 | CE2 | | 246 | 31.549 | 18.236 | 68.835 | 1.00 19.88 | AAAA |
| MOTA | 1957 | CZ | PHE | 246 | 29.233 | 19.176 | 73.712 | 1.00 23.38 | AAAA |
| ATOM | 1958 | C | PHE | 246 | 28.867 | 20.312 | 74.002 | 1.00 29.15 | AAAA |
| ATOM | 1959 | 0 | PHE | 247 | 30.410 | 18.682 | 74.094 | 1.00 29.73 | AAAA |
| ATOM | 1960 | N | GLU | 247 | 31.395 | 19.481 | 74.841 | 1.00 28.10 | AAAA |
| ATOM | 1961 | CA | GLU | 247 | 31.912 | 18.726 | 76.074 | 1.00 35.75 | AAAA |
| ATOM | 1962 | CB | GLU | | 30.972 | 18.707 | 77.286 | 1.00 60.78 | AAAA |
| ATOM | 1963 | CG | GLU | 247 | 29.700 | | 77.077 | 1.00 70.07. | AAAA |
| MOTA | 1964 | CD | GLU | 247 | 28.913 | 18.220 | | 1.00 79.95 | AAAA |
| MOTA | 1965 | | GLU | 247 | 29.481 | 16.920 | | 1.00 76.80 | AAAA |
| ATOM | 1966 | | GLU | 247 | 32.554 | 19.741 | | 1.00 28.90 | AAAA |
| MOTA | 1967 | С | GLU | 247 | | 18.946 | | 1.00 23.67 | AAAA |
| ATOM | 1968 | 0 | GLU | 247 | 33.490 32.531 | 20.891 | | 1.00 25.02 | AAAA |
| MOTA | 1969 | N | PRO | 248 | | 22.003 | | | AAAA |
| MOTA | 1970 | CD | PRO | 248 | 31.574 | 21.249 | | | AAAA |
| ATOM | 1971 | CA | PRO | 248 | 33.566 | | | | AAAA |
| ATOM | 1972 | CB | PRO | 248 | 33.050 | | | | AAAA |
| ATOM | 1973 | CG | PRO | | 31.551 | | | | AAAA |
| ATOM | 1974 | С | PRO | | 34.968 | | | | AAAA |
| ATOM | 1975 | 0 | PRO | | 35.132 | | | | AAAA |
| ATOM | 1976 | N | GLU | 249 | 35.965 | | | | AAAA |
| ATOM | 1977 | CA | GLU | | 37.366 | | | | AAAA |
| ATOM | 1978 | | GLU | | 38.275 | 20.166 | | 40 | AAAA |
| MOTA | 1979 | | GLU | | 38.046 | | | | AAAA |
| ATOM | 1980 | | GLU | | 39.005 | | 71.445 | 1.00 29.15 | , was |

ATOM

| | | 053 | CT II | 249 | 30 | .071 | 17.770 | 70:199 | 1.00 27.62 | AÁAA |
|------|--------|-----|-------|------------|----|------------------|----------|----------|------------|------|
| ATOM | 1981 | OE1 | | 249 | | .694 | 17.004 | 72.161 | 1.00 26.19 | AAAA |
| MOTA | 1982 | OE2 | | 249 | | .692 | 22.561 | 71.786 | 1.00 26.04 | AAAA |
| MOTA | 1983 | - | GLU | 249 | - | .582 | 23.271 | 72.262 | 1.00 26.39 | AAAA |
| MOTA | 1984 | | GLU | 250 | - | .953 | 22.921 | 70.744 | 1.00 23.83 | AAAA |
| MOTA | 1985 | | VAL | 250 | | .151 | 24197 | 70.086 | 1.00 19.67 | AAAA |
| MOTA | 1986 | | VAL | 250 | _ | .438 | 24.178 | 69.210 | 1.00 20.88 | AAAA |
| MOŢA | 1987 | | VAL | 250 | | .348 | 23.117 | 68.128 | 1.00 18.18 | AAAA |
| MOTA | 1988 | CG1 | | | | .647 | 25.530 | 68.591 | 1.00 16.71 | AAAA |
| MOTA | 1989 | CG2 | | .250 | | .946 | 24.483 | 69.207 | 1.00 20.78 | AAAA |
| MOTA | 1990 | - | VAL | 250 | | .299 | 23.556 | 68.746 | 1.00 19.60 | AAAA |
| ATOM | 1991 | - | VAL | 250 | | .633 | 25.757 | 69.000 | 1.00 18.75 | AAAA |
| MOTA | 1992 | N | TYR | 251 | | .497 | 26.109 | 68.153 | 1.00 22.44 | AAAA |
| MOTA | 1993 | CA | TYR | 251 | | .261 | 26.437 | 69.022 | 1.00 16.57 | AAAA |
| MOTA | 1994 | CB | TYR | 251 | | .207 | 27.856 | 69.575 | 1.00 22.36 | AAAA |
| ATOM | 1995 | CG | TYR | 251 | | 2.654 | 28.896 | 68.823 | 1.00 18.12 | AAAA |
| MOTA | 1996 | CD1 | | 251 | | .612 | 30.185 | 69.308 | 1.00 20.40 | AAAA |
| ATOM | 1997 | CEl | | 251 | | 3.715 | 28.160 | 70.842 | 1.00 20.04 | AAAA |
| MOTA | 1998 | | TYR | 251 | | 3.676 | 29.475 | 71.349 | 1.00 16.60 | AAAA |
| ATOM | 1999 | CE2 | TYR | 251 | | 3.128 | 30.473 | 70.573 | 1.00 14.68 | AAAA |
| MOTA | 2000 | CZ | TYR | 251 | | 3.100 | 31.780 | 71.011 | 1.00 21.79 | AAAA |
| MOTA | 2001 | OH | TYR | 251 | | 1.811 | 27.294 | 67.236 | 1.00 20.28 | AAAA |
| MOTA | 2002 | C | TYR | 251 | | 5.695 | 28.107 | 67.525 | 1.00 19.91 | AAAA |
| MOTA | 2003 | 0 | TYR | 251 | _ | 1.097 | 27.360 | 66.109 | 1.00 17.90 | AAAA |
| MOTA | 2004 | N | LEU | 252 | | 1.216 | 28.466 | 65.161 | 1.00 18.58 | AAAA |
| MOTA | 2005 | CA | LEU | 252 | | 4.679 | 28.001 | 63.767 | 1.00 17.55 | AAAA |
| MOTA | 2006 | CB | LEU | 252 | | 6.028 | 27.290 | 63.718 | 1.00 23.36 | AAAA |
| MOTA | 2007 | CG | LEU | 252 | | 5.819 | 25.820 | 64.017 | 1.00 27.78 | AAAA |
| MOTA | 2008 | | LEU | 252 | | 6.631 | 27.440 | 62.331 | 1.00 27.29 | AAAA |
| ATOM | 2009 | | LEU | 252 | | 2.816 | 29.049 | 65.052 | 1.00 15.49 | AAAA |
| MOTA | 2010 | C | LEU | 252 252 | | 1.819 | 28.320 | 65.120 | 1.00 18.82 | AAAA |
| MOTA | 2011 | 0 | LEU | | | 2.756 | 30.360 | 64.891 | 1.00 16.80 | AAAA |
| MOTA | 2012 | N | LEU | 253 | | 1.498 | 31.105 | 64.817 | 1.00 17.50 | AAAA |
| MOTA | 2013 | CA | LEU | 253 253 | _ | 1.379 | 31.987 | 66.073 | 1.00 15.49 | AAAA |
| ATOM | 2014 | CB | LEU | 253 | | 0.326 | 33.085 | 66.165 | 1.00 17.75 | AAAA |
| ATOM | 2015 | CG | LEU | 253 | _ | 8.946 | 32.438 | 66.172 | 1.00 20.85 | AAAA |
| ATOM | 2016 | | LEU | 253 | | 0.536 | 33.897 | 67.464 | 1.00 19.05 | AAAA |
| MOTA | 2017 | | LEU | 253 | | 1.516 | 31.985 | 63.580 | 1.00 20.22 | AAAA |
| MOTA | 2018 | С | LEU | 253 | | 2.474 | 32.727 | 63.371 | 1.00 18.14 | AAAA |
| MOTA | 2019 | 0 | LEU | 254 | | 0.466 | 31.913 | 62.765 | 1.00 16.50 | AAAA |
| MOTA | 2020 | N | GLN | 254 | | 0.411 | 32.730 | 61.556 | 1.00 16.48 | AAAA |
| ATOM | 2021 | CA | GLN | 254 | 7 | 0.085 | 31.863 | 60.312 | 1.00 25.58 | AAAA |
| MOTA | 2022 | CB | GLN | 254 | | 8.647 | 31.798 | 59.871 | 1.00 36.40 | AAAA |
| MOTA | 2023 | CG | GLN | 254 | | 8.337 | 32.728 | 58.701 | 1.00 33.18 | AAAA |
| ATOM | 2024 | CD | GLN | 254 | | 8.744 | 32.487 | | 1.00 21.05 | AAAA |
| MOTA | 2025 | | GLN | 254 | 5 | 7.613 | 33.799 | | 1.00 22.85 | AAAA |
| MOTA | . 2026 | | GLN | 254 | | 9.384 | 33.816 | | 1.00 16.12 | AAAA |
| MOTA | 2027 | C | GLN | 254 | | 8.282 | 33.577 | | 1.00 13.97 | AAAA |
| MOTA | 2028 | | GLN | 255 | | 9.768 | | | 1.00 14.42 | AAAA |
| ATOM | 2029 | N | LEU | 255 | | 8.988 | | | 1.00 17.99 | AAAA |
| MOTA | 2030 | CA | LEU | 255 | | 9.834 | | | 1.00 20.68 | AAAA |
| MOTA | 2031 | CB | LEU | 255 | | 0.240 | | | | AAAA |
| MOTA | 2032 | CG | LEU | 255 | | 1.446 | | | 1.00 29.36 | AAAA |
| ATOM | 2033 | | LEU | 255 | | 9.042 | | . 64.900 | 1.00 14.80 | AAAA |
| MOTA | 2034 | | LEU | 255 | | 28.541 | | | 1.00 19.32 | AAAA |
| MOTA | 2035 | C | LEU | | | 28.838 | | | 1.00 21.23 | AAAA |
| MOTA | 2036 | 0 | LEU | 255 | | 27.827 | | | 1.00 17.21 | AAAA |
| MOTA | 2037 | N | GLY | 256 | | 27.347 | | | | AAAA |
| MOTA | 2038 | | GLY | 256 256 | | 26.413 | | | 1.00 17.31 | AAAA |
| MOTA | 2039 | | GLY | 256 | | 25.717 | | | 1.00 15.62 | AAAA |
| MOTA | 2040 | | GLY | 256 | | 25.717 26.389 | | | 1.00 19.72 | AAAA |
| ATOM | 2041 | | THR | 257 | | 25.536 | | | 1.00 19.88 | AAAA |
| ATOM | 2042 | | | 257 | | 25.330 26.242 | | | 1.00 14.02 | AAAA |
| ATOM | 2043 | | | | | 26.538 | | | 1.00 17.58 | AAAA |
| MOTA | 2044 | | 1 THR | | | 26.536 27.543 | | | 1.00 19.67 | AAAA |
| MOTA | 2045 | | 2 THR | | | 27.343 24.199 | | | | AAAA |
| ATCM | 2046 | C | THR | 257 | | 44.173 | , 40.031 | | | • |
| | • | | • | • | | | | | | |

| | -047 | ^ | mu: | 257 | 2. | 3 403 | 41.545 | 58.266 | 1.00 14.59 | AAAA |
|--------|------|-----|-------|-----|----|---------|--------|----------|------------|-------|
| MOTA | 2047 | 0 | THR | | | 3.927 | 39.639 | 57.213 | 1.00 16.56 | AAAA |
| ATOM | 2048 | N | ASP | 258 | | | 39.646 | 56.525 | 1.00 16.39 | AAAA |
| MOTA | 2049 | CA | ASP | 258 | | 2.651 | | | 1.00 18.38 | AAAA |
| MOTA | 2050 | CB | ASP | 258 | | 2.604 | 38.611 | 55.388 | | AAAA |
| ATOM | 2051 | CG | ASP | 258 | | 3.037 | 37.229 | 55.811 | 1.00 25.85 | |
| ATOM - | 2052 | OD1 | ASP | 258 | 2 | 3.222 | 36.995 | 57.022 | 1.00 22.32 | AAAA |
| | | OD2 | | 258 | | 3.187 | 36.370 | 54.909 | 1.00 18.12 | AAAA |
| MOTA | 2053 | | | 258 | | 1.396 | 39.563 | 57.397 | 1.00 21.25 | AAAA |
| ATOM | 2054 | C | ASP | | - | 0.300 | 39.781 | 56.897 | 1.00 22.52 | AAAA |
| MOŢA | 2055 | 0 | ASP | 258 | | | 39.172 | 58.680 | 1.00 18.17 | AAAA |
| ATOM | 2056 | N | PRO | 259 | | 1.510 | | | 1.00 25.88 | AAAA |
| MOTA | 2057 | CD | PRO | 259 | | 2.614 | 38.528 | 59.422 | 1.00 21.24 | AAAA |
| ATOM | 2058 | CA | PRO | 259 | _ | 0.281 | 39.139 | 59.482 | | AAAA |
| ATOM | 2059 | СВ | PRO | 259 | | 0.710 | 38.363 | 60.735 - | 1.00 21.18 | |
| | 2060 | CG | PRO | 259 | 2 | 2.174 | 38.707 | 60.846 | 1.00 36.11 | AAAA |
| ATOM | | | PRO | 259 | | 9.705 | 40.534 | 59.820 | 1.00 20.88 | AAAA |
| ATOM | 2061 | C | | 259 | | 8.572 | 40.647 | 60.280 | 1.00 19.25 | -AAAA |
| ATOM | 2062 | 0 | PRO | | | 0.473 | 41.591 | 59.571 | 1.00 18.75 | AAAA |
| MOTA | 2063 | N | LEU | 260 | | | 42.949 | 59.875 | 1.00 22.16 | AAAA |
| MOTA | 2064 | CA | LEU | 260 | | 0.023 | | 59.778 | 1.00 20.35 | AAAA |
| ATOM | 2065 | CB | LEU | 260 | | 1.202 | 43.935 | | 1.00 21.82 | AAAA |
| ATOM | 2066 | CG | LEU | 260 | | 2.403 | 43.640 | 60.682 | | AAAA |
| | 2067 | | LEU | 260 | 2 | 3.604 | 44.486 | 60.253 | 1.00 18.57 | |
| MOTA | 2068 | | LEU | 260 | 2 | 2.032 | 43.873 | 62.123 | 1.00 19.18 | AAAA |
| ATOM | | | | 260 | | 8.876 | 43.469 | 59.014 | 1.00 24.16 | AAAA |
| MOTA | 2069 | C | LEU | | | 8.742 | 43.144 | 57.826 | 1.00 21.69 | AAAA |
| MOTA | 2070 | 0 | LEU | 260 | | 8.049 | 44.300 | 59.634 | 1.00 19.54 | AAAA |
| MOTA | 2071 | N | LEU | 261 | | | 44.913 | 58.965 | 1.00 17.34 | AAAA |
| ATOM | 2072 | CA | LEU | 261 | | 6.903 | | 59.892 | 1.00 19.96 | AAAA |
| ATOM | 2073 | CB | LEU | 261 | | 6.285 | 45.967 | | 1.00 29.99 | AAAA |
| ATOM | 2074 | CG | LEU | 261 | | .5.204 | 46.879 | 59.300 | | AAAA |
| ATOM | 2075 | | LEU | 261 | 1 | 4.080 | 46.040 | 58.732 | 1.00 33.66 | |
| | 2076 | | LEU | 261 | 3 | 4.682 | 47.819 | 60.376 | 1.00 44.71 | AAAA |
| MOTA | _ | | LEU | 261 | 1 | 7.262 | 45.550 | 57.620 | 1.00 18.11 | AAAA |
| MOTA | 2077 | C | | 261 | | 6.539 | 45.386 | 56.634 | 1.00 19.02 | AAAA |
| MOTA | 2078 | 0 | LEU | | | 18.391 | 46.249 | 57.566 | 1.00 22.68 | AAAA |
| MOTA | 2079 | N | GLU | 262 | | 18.802 | 46.921 | 56.338 | 1.00 18.46 | AAAA |
| ATOM | 2080 | CA | GLU | 262 | | | 47.965 | 56.641 | 1.00 22.01 | AAAA |
| ATOM | 2081 | CB | GLU | 262 | | 19.875 | | 57.443 | 1.00 22.94 | AAAA |
| ATOM | 2082 | CG | GLU | 262 | | 19.365 | 49.136 | | 1.00 23.11 | AAAA |
| ATOM | 2083 | CD | GLU | 262 | | 19.434 | 48.902 | 58.927 | 1.00 23.11 | AAAA |
| MOTA | 2084 | | GLU | 262 | : | 19.668 | 47.748 | 59.357 | 1.00 24.58 | |
| | 2085 | | GLU | 262 | | 19.238 | 49.883 | 59.667 | 1.00 27.06 | AAAA |
| ATOM | | C | GLU | 262 | | 19.281 | 46.034 | 55.197 | 1.00 25.65 | AAAA |
| ATOM | 2086 | | | 262 | | 19.446 | 46.510 | 54.070 | 1.00 25.49 | AAAA |
| MOTA | 2087 | 0 | GLU | | | 19.501 | | 55.467 | 1.00 22.45 | AAAA |
| MOTA | 2088 | N | ASP | 263 | | 19.959 | 43.851 | 54.418 | 1.00 15.93 | AAAA |
| MOTA | 2089 | CA | ASP | 263 | | | 42.859 | 54.988 | 1.00 18.99 | AAAA |
| MOTA | 2090 | CB | ASP | 263 | | 20.981 | 42.081 | 53.907 | 1.00 22.21 | AAAA |
| MOTA | 2091 | CG | ASP | 263 | | 21.706 | | | | |
| ATOM | 2092 | OD1 | ASP | 263 | | 22.876 | 41.730 | | 1.00 25.02 | |
| MOTA | 2093 | | ASP | 263 | | 21.112 | 41.809 | | | |
| | 2094 | C | ASP | 263 | | 18.733 | 43.165 | | | |
| MOTA | 2095 | ō | ASP | 263 | | 18.012 | 42.419 | 54.519 | | |
| ATOM | | | TYR | 264 | | 18.500 | | | 1.00 25.21 | AAAA |
| ATOM | 2096 | N | | | | 17.339 | | | 1.00 29.92 | AAAA |
| MOTA | 2097 | CA | TYR | 264 | | 17.077 | | | | AAAA |
| MOTA | 2098 | CB | TYR | 264 | | | | | | AAAA |
| MOTA | 2099 | CG | TYR | 264 | | 17.910 | | | | AAAA |
| ATOM | 2100 | CD | TYR | 264 | | 17.677 | | | | |
| ATOM | 2101 | | LTYR | 264 | | 18.420 | 41.930 | | | |
| ATOM | 2102 | | TYR | 264 | | 18.915 | 44.286 | | | |
| | 2103 | CE | | 264 | | 19.670 | 43.975 | 47.788 | 1.00 74.50 | |
| ATOM | | | | 264 | | 19.415 | | | 1.00 72.57 | AAAA |
| MOTA | 2104 | CZ | TYR | | | 20.154 | | | 1.00 71.96 | AAAA |
| atom | 2105 | OH | TYR | 264 | | 17.445 | | | | AAAA |
| MOTA | 2106 | C | TYR | 264 | | | | | | AAAA |
| ATOM | 2107 | 0 | TYR | 264 | | 16.448 | | | | - |
| ATOM | 2108 | | LEU | 265 | | 1.8.639 | | | | |
| MOTA | 2109 | | | 265 | | 18.753 | | | | |
| | 2110 | | | 265 | | 20.186 | | | | - |
| ATOM | 2111 | | | 265 | | 20.509 | | | | |
| ATOM | | | | | | 21.847 | | | 1.00 44.38 | AAAA |
| MOTA | 2112 | | 1 LEU | 233 | | | | • | • | • |
| | | | | | | | | | | |

| | | | | | • | | | | |
|--------------|--------------|----------|------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| | 0113 | CD3 | 1 511 | 265 | 19.422 | 38.990 | 48.603 | 1.00 46.72 | AAAA |
| MOTA | 2113 2114 | CD2 C | LEU | 265 | 18.209 | 38.585 | 52.447 | 1.00 22.33 | AAAA |
| ATOM | | 0 | LEU | 265 | 18.279 | 37.364 | 52.348 | 1.00 23.48 | AAAA |
| ATOM | 2115 2116 | N | SER | 266 | 17.677 | 39.194 | 53.508 | 1.00 17.50 | AAAA |
| ATOM | 2117 | CA | SER | 266 | 17.055 | 38.398 | 54.569 | 1.00 19.69 | AAAA |
| MOTA | 2117 | CB | SER | 266 | 17.912 | 38.314 | 55.845 | 1.00 20.73 | AAAA |
| MOTA | 2119 | OG. | SER | 266 | 17.696 | 39.442 | 56.684 | 1.00 22.81 | AAAA |
| MOTA MOTA | 2120 | C . | SER | 266 | 15.739 | 39.048 | 54.950 | 1.00 19.75 | AAAA |
| ATOM | 2121 | Ö | SER | 266 | 15.572 | 40.265 | 54.840 | 1.00 23.66 | AAAA |
| ATOM | 2122 | N | LYS | 267 | 14.799 | 38.229 | 55.402 | 1.00 18.40 | AAAA AAAA |
| MOTA | 2123 | CA | LYS | 267 | 13.527 | 38.759 | 55.851 | 1.00 20.64 1.00 20.96 | AAAA |
| MOTA | 2124 | CB | LYS | 267 | 12.397 | 37.787 | 55.513 54.025 | 1.00 25.60 | AAAA |
| ATOM | 2125 | CG | LYS | 267 | 12.269 | 37.536 | 53.259 | 1.00 23.00 | AAAA |
| ATOM | 2126 | CD | LYS | 267 | 12.095 | 38.823 38.540 | 51.772 | 1.00 38.49 | AAAA |
| ATOM | 2127 | CE | LYS | 267 | 11.985 | 39.793 | 50.991 | 1.00 33.11 | AAAA |
| MOTA | 2128 | NZ | LYS | 267 | 11.954 13.601 | 38.987 | 57.365 | 1.00 20.63 | AAAA |
| MOTA | 2129 | C | LYS | 267 | 12.584 | 39.192 | 58.017 | 1.00 25.38 | AAAA |
| MOTA | 2130 | 0 | LYS | 267 268 | 14.814 | 38.937 | 57.915 | 1.00 18.98 | AAAA |
| MOTA | 2131 | N | PHE | 268 | 15.034 | 39.182 | 59.345 | 1.00 18.50 | AAAA |
| MOTA | 2132 | CA CB | PHE PHE | 268 | 16.328 | 38.510 | 59.833 | 1.00 20.91 | AAAA |
| MOTA | 2133 2134 | CG | PHE | 268 | 16.252 | 37.006 | 59.967 | 1.00 16.96 | AAAA |
| MOTA | 2134 | | PHE | 268 | 17.374 | 36.290 | 60.415 | 1.00 16.61 | AAAA |
| MOTA | 2135 | | PHE | 268 | 15.081 | 36.303 | 59.682 | 1.00 18.13 | AAAA |
| ATOM ATOM | 2137 | | PHE | 268 | 17.331 | | 60.581 | 1.00 14.81 | AAAA AAAA |
| MOTA | 2138 | | PHE | 268 | 15.027 | | 59.849 | 1.00 17.45 | AAAA |
| ATOM | 2139 | CZ | PHE | 268 | 16.144 | | 60.296 | 1.00 16.01 1.00 18.33 | AAAA |
| MOTA | 2140 | С | PHE | 268 | 15.179 | | 59.510 | 1.00 18.33 | AAAA |
| ATOM | 2141 | 0 | PHE | 268 | 15.733 | 41.371 | 58.644 60.613 | 1.00 21.04 | AAAA |
| ATOM | 2142 | N | ASN | 269 | 14.679 | | 60.859 | 1.00 22.89 | AAAA |
| ATOM | 2143 | CA | ASN | 269 | 14.763 | | 60.940 | 1.00 20.55 | AAAA |
| ATOM | 2144 | CB | ASN | 269 | 13.365 12.551 | | | 1.00 26.13 | AAAA |
| MOTA | 2145 | CG | ASN | 269 | 13.060 | | 58.571 | 1.00 29.17 | AAAA |
| MOTA | 2146 | | ASN | 269 269 | 11.268 | | 59.860 | 1.00 28.26 | AAAA |
| MOTA | 2147 | | ASN ASN | 269 | 15.493 | | 62.159 | 1.00 19.00 | AAAA |
| ATOM | 2148 2149 | С 0 | ASN | 269 | 14.984 | | 63.019 | 1.00.21.85 | AAAA |
| ATOM | 2150 | N | LEU | 270 | 16.695 | 42.435 | 62.298 | 1.00 17.71 | AAAA |
| ATOM ATOM | 2151 | CA | LEU | 270 | 17.441 | | 63.521 | 1.00 18.57 | AAAA AAAA |
| MOTA | 2152 | СВ | LEU | 270 | 18.441 | | 63.712 | 1.00 18.95 | AAAA |
| MOTA | 2153 | CG | LEU | 270 | 17.945 | | 63.631 | 1.00 20.54 1.00 14.19 | AAAA |
| ATOM | 2154 | CD1 | LEU | 270 | 19.070 | | 64.152 | 1.00 19.05 | AAAA |
| ATOM | 2155 | CD2 | LEU | 270 | 16.679 | | 64.465 63.583 | 1.00 22.83 | AAAA |
| ATOM | 2156 | С | LEU | 270 | 18.203 | | 62.560 | 1.00 18.25 | AAAA |
| MOTA | 2157 | 0 | LEU | 270 | 18.409 | | 64.799 | 1.00 20.95 | AAAA |
| MOTA | 2158 | N. | | 271 | 18.621 19.414 | | | 1.00 18.28 | AAAA |
| MOTA | 2159 | CA | SER | 271 | 18.985 | | | 1.00 18.73 | AAAA |
| MOTA | 2160 | CB | SER | 271 271 | 19.34 | _ | | 1.00 22.28 | AAAA |
| MOTA | 2161 | OG | SER | 271 | 20.87 | | | 1.00 19.98 | AAAA |
| MOTA | 2162 | C O | SER | 271 | 21.12 | | 65.537° | 1.00 18.82 | AAAA |
| MOTA | 2163 2164 | N | ASN | 272 | 21.82 | | | 1.00 16.17 | AAAA |
| MOTA | 2165 | CA | ASN | 272 | 23.27 | 0 45.695 | | 1.00 20 70 | AAAA AAAA |
| MOTA MOTA | 2166 | CB | ASN | 272 | 24.17 | 6 46.903 | | | AAAA |
| MOTA | 2167 | CG | | 272 | 24.16 | | 63.483 | | AAAA |
| MOTA | 2168 | | 1 ASN | 272 - | 24.70 | | | | AAAA |
| ATOM | 2169 | | 2 ASN | 272 | 23.57 | | | | AAAA |
| ATOM | 2170 | | ASN | 272 | 23.58 | | | | AAAA |
| MOTA | 2171 | _ | ASN | 272 | 24.54 | | | | AAAA |
| MOTA | 2172 | | VAL | 273 | 22.83 | | | | AAAA |
| MOTA | 2173 | CA | | 273 | 23.05 | | | | AAAA |
| ATOM | 2174 | | | 273 | 22.34 22.44 | | | | AAAA |
| ATOM | 2175 | | 1 VAL | | 22.44 | | | 1.00 34.73 | AAAA |
| ATOM | 2176 | | 2 VAL | | 23.03 | | | 1.00 22.06 | AAAA |
| ATOM | 2177 | | VAL | | 23.24 | | | | AAAA |
| 3 TOM | 7178 | 0 | VAL | 213 | ~~ | | • | | • |

| | | | | 274 | 21.601 | 43.747 | 68.713 | 1.00 21.79 | AAAA |
|--------------|--------------|---------|--------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| MOTA | 2179 | И | ALA | 274 | 21.207 | 42.383 | 69.035 | 1.00 21.31 | AAAA |
| MOTA | 2180 | CA | ALA ALA | 274 | 19.806 | 42.092 | 68.475 | 1.00 18.95 | AAAA |
| ATOM | 2181 | CB | ALA | 274 | 22.259 | 41.451 | 68.400 | 1.00 17.83 | AAAA |
| MOTA | 2182 | C 0 | ALA | 274 | 22.569 | 40.389 | 68.947 | 1.00 20.38 | AAAA |
| ATOM | 2183 | И | PHE | 275 | 22.798 | 41.859 | 67.245 | 1.00 16.01 | AAAA |
| MOTA | 2184 2185 | CA | PHE | 275 | 23.828 | 41.089 | 66.536 | 1.00 16.46 | AAAA |
| MOTA | 2186 | CB | PHE | 275 | 24.220 | 41.835 | 65.253 | 1.00 24.56 | AAAA |
| ATOM | 2187 | CG | PHE | 275 | 25.363 | 41.222 | 64.492 | 1.00 23.01 | AAAA |
| MOTA MOTA | 2188 | CD1 | | 275 | 25.209 | 40.035 | 63.788 | 1.00 23.88 | AAAA |
| ATOM | 2189 | | PHE | 275 | 26.590 | 41.877 | 64.443 | 1.00 22.40 | AAAA AAAA |
| ATOM | 2190 | | PHE | 275 | 26.266 | 39.510 | 63.038 | 1.00 28.74 | AAAA |
| MOTA | 2191 | | PHE | 275 | 27.654 | 41.365 | 63.700 | 1.00 35.03 1.00 24.63 | AAAA |
| ATOM | 2192 | CZ | PHE | 275 | 27.489 | 40.181 | 62.996 67.469 | 1.00 25.06 | AAAA |
| ATOM | 2193 | C | PHE | 275 | 25.030 | 40.964 | 67.632 | 1.00 19.71 | AAAA |
| MOTA | 2194 | 0 | PHE | 275 | 25.619 | 39.888 42.080 | 68.101 | 1.00 17.49 | AAAA |
| MOTA | 2195 | N | LEU | 276 | 25.366 26.482 | 42.000 | 69.030 | 1.00 24.23 | AAAA |
| MOTA | 2196 | CA | LEU | 276 | 26.736 | 43.606 | 69.416 | 1.00 20.44 | AAAA |
| MOTA | 2197 | СВ | LEU | 276 | 28.001 | 43.967 | 70.211 | 1.00 39.65 | AAAA |
| MOTA | 2198 | CG | LEU | 276 276 | 27.948 | 45.447 | 70.589 | 1.00 29.65 | AAAA |
| ATOM | 2199 | | LEU LEU | 276 | 28.102 | 43.143 | 71.460 | 1.00 32.41 | AAAA |
| MOTA | 2200 | | LEU | 276 | 26.180 | 41.278 | 70.262 | 1.00 18.86 | AAAA |
| MOTA | 2201 | C 0 | LEU | 276 | 27.045 | 40.529 | 70.727 | 1.00 17.99 | AAAA |
| MOTA | 2202 2203 | И | LYS | 277 | 24.968 | 41.374 | 70.805 | 1.00 19.67 | AAAA |
| MOTA MOTA | 2204 | CA | LYS | 277 | 24.644 | 40.552 | 71.964 | 1.00 21.33 | AAAA |
| ATOM | 2205 | CB. | LYS | 277 | 23.265 | 40.888 | 72.532 | 1.00 23.84 | AAAA |
| ATOM | 2206 | CG | LYS | 277 | 23.247 | 42.126 | 73.366 | 1.00 40.87 | AAAA AAAA |
| ATOM | 2207 | CD | LYS | 277 | 22.069 | 42.086 | 74.325 | 1.00 54.73 1.00 58.85 | AAAA |
| ATOM | 2208 | CE | LYS | 277 | 22.172 | 40.884 | 75.254 | 1.00 55.34 | AAAA |
| ATOM | 2209 | NZ | LYS | 277 | 21.051 | 40.844 | 76.228 71.660 | 1.00 33.34 | AAAA |
| ATOM | 2210 | С | LYS | 277 | 24.695 | 39.068 38.264 | 72.513 | 1.00 22.12 | AAAA |
| ATOM | 2211 | 0 | LYS | 277 | 25.074 | 38.700 | 70.441 | 1.00 20.23 | AAAA |
| ATOM | 2212 | N | ALA | 278 | 24.311 24.325 | 37.291 | 70.039 | 1.00 17.06 | AAAA |
| ATOM | 2213 | CA | ALA | 278 278 | 23.798 | 37.154 | 68.589 | 1.00 19.27 | AAAA |
| MOTA | 2214 | CB | ALA | 278 278 | 25.760 | 36.767 | 70.127 | 1.00 16.94 | AAAA |
| MOTA | 2215 | C | ALA | 278 | 26.035 | 35.676 | 70.648 | 1.00 14.93 | AAAA |
| MOTA | 2216 | O N | ALA PHE | 279 | 26.679 | 37.564 | 69.606 | 1.00 18.88 | AAAA |
| MOTA | 2217 2218 | N CA | PHE | 279 | 28.099 | 37.231 | 69.626 | 1.00 21.01 | AAAA |
| ATOM | 2219 | CB | PHE | 279 | 28.880 | 38.392 | 68.998 | 1.00 16.79 | AAAA |
| ATOM ATOM | 2220 | CG | ?HE | 279 | 30.370 | 38.264 | 69.120 | 1.00 20.23 | AAAA |
| MOTA | 2221 | | PHE | 279 | 31.062 | 37.272 | 68.423 | 1.00 21.61 | AAAA AAAA |
| MOTA | 2222 | | PHE | 279 | 31.088 | 39.159 | 69.905 | 1.00 23.24 1.00 30.98 | AAAA |
| ATOM | 2223 | | PHE | 279 | 32.461 | 37.185 | 68.509 | 1.00 30.98 | AAAA |
| ATOM | 2224 | CE2 | PHE | 279 | 32.480 | 39.081 | 69.995 | 1.00 24.02 | AAAA |
| ATOM | 2225 | CZ | PHE | 279 | 33.169 | 38.095 | 69.295 71.067 | 1.00 35.27 | AAAA |
| ATOM | 2226 | С | PHE | 279 | 28.576 | 36.995 36.016 | 71.362 | 1.00 16.30 | AAAA |
| MOTA | 2227 | 0 | PHE | 279 | 29.275 | 37.898 | 71.962 | 1.00 22.30 | AAAA |
| MOTA | 2228 | N | ASN | 280 | 28.194 28.599 | 37.777 | 73.352 | | AAAA |
| MOTA | 2229 | CA | ASN | 280 | 28.391 | 39.109 | 74.080 | 1.00 27.17 | AAAA |
| MOTA | 2230 | CB | ASN | 280 280 | 29.344 | 40.183 | | 1.00 20.88 | AAAA |
| MOTA | 2231 | CG | NSA NSA J | 280 | 30.503 | 39.897 | | 1.00 22.95 | AAAA |
| ATOM | 2232 | | ASN | 280 | 28.875 | 41.421 | | 1.00 27.85 | AAAA |
| ATOM | 2233 | C | ASN | 280 | 27.928 | 36.636 | 74.095 | 1.00 23.01 | AAAA |
| ATOM | 2234 2235 | 0 | ASN | 280 | 28.510 | 36.062 | | 1.00 21.91 | AAAA |
| MOTA | 2236 | N | ILE | 281 | 26.711 | 36.300 | | 1.00 18.74 | AAAA |
| MOTA | 2237 | CA | ILE | 281 | 26.005 | 35.179 | | 1.00 18.37 | AAAA LAKK |
| MOTA MOTA | 2238 | CB | ILE | 281 | 24.566 | 35.067 | | | AAAA AAAA |
| ATOM | 2239 | | 2 ILE | 281 | 23.977 | 33.725 | | | AAAA |
| MOTA | 2240 | | 1 ILE | 281 | 23.710 | 36.206 | | | AAAA |
| ATOM | 2241 | CD: | 1 ILE | 281 | 22.279 | 36.193 | | | AAAA |
| ATOM | 2242 | | ILE | 281 | 26.743 | 33.876 | | | AAAA |
| ATOM | 2243 | 0 | ILE | 281 | 26.830 | 32.973 | | | AAAA |
| ATOM | 2244 | N | VAL | 282 | 27.258 | 33.765 | 12.144 | 2.00 27.72 | • |
| | | | • | • | • | | | | |

| | | | | | 27.976 | 32.553 | 72.352 | 1.00 14.89 | AAAA |
|------|--------|------|-------|-----|--------|----------|----------|--------------|-------|
| ATOM | 2245 | CA | VAL | 282 | | | 70.852 | 1.00 18.50 | AAAA |
| ATOM | 2246 | CB | VAL | 282 | 28.359 | 32.565 | 70.552 | 1.00 20.73 | AAAA |
| MOTA | 2247 | CG1 | VAL | 282 | 29.342 | 31.440 | 70.307 | 1.00 17.49 | AAAA |
| ATOM | 2248 | CG2 | VAL | 282 | 27.105 | 32.363 | 69.994 | 1.00 17.49 | AAAA |
| ATOM | 2249 | C | VAL | 282 | 29.241 | 32.433 | 73.198 | | |
| | 2250 | ō | VAL | 282 | 29.568 | 31.360 | 73.715 | 1.00 25.80 | AAAA |
| ATOM | | N | ARG | 283 | 29.935 | 33.549 | 73.361 | 1.00 19.14 | AAAA |
| MOTA | 2251 | | ARG | 283 | 31.161 | 33.548 | 74.150 | 1.00 23.51 | AAAA |
| MOTA | 2252 | CA | | 283 | 31.851 | 34.898 | 74.023 | 1.00 20.64 | AAAA |
| MOTA | 2253 | CB | ARG | | 32.338 | 35.200 | 72.607 | 1.00 19.65 | AAAA |
| ATOM | 2254 | CG | ARG | 283 | 32.754 | 36.645 | 72.474 | 1.00 25.70 | AAAA |
| ATOM | 2255 | CD | ARG | 283 | | 36.944 | 73.215 | 1.00 36.05 | AAAA |
| MOTA | 2256 | NE | ARG | 283 | 33.970 | 38.147 | 73.681 | 1.00 34.61 | AAAA |
| MOTA | 2257 | CZ | ARG | 283 | 34.277 | | 73.488 | 1.00 35.23 | AAAA |
| MOTA | 2258 | NHl | ARG | 283 | 33.448 | 39.169 | 74.326 | 1.00 29.30 | AAAA |
| ATOM | 2259 | NH2 | ARG | 283 | 35.419 | 38.332 | | 1.00 25.44 | AAAA |
| MOTA | 2260 | С | ARG | 283 | 30.911 | 33.219 | 75.622 | 1.00 23.44 | AAAA |
| | 2261 | ō | ARG | 283 | 31.754 | 32.600 | 76.272 | | AAAA |
| MOTA | 2262 | N | GLU | 284 | 29.765 | 33.632 | 76.151 | 1.00 26.79 | |
| MOTA | 2263 | CA | GLU | 284 | 29.462 | 33.338 | 77.553 | 1.00 31.77 | AAAA |
| MOTA | | CB | GLU | 284 | 28.243 | 34.115 | 78.033 | 1.00 30.96 | AAAA. |
| MOTA | 2264 | | GLU | 284 | 28.399 | 35.605 | 77.957 | 1.00 50.56 | AAAA |
| MOTA | 2265 | CG | | 284 | 27.137 | 36.320 | 78.365 | 1.00 63.75 | AAAA |
| MOTA | 2266 | CD | GLU | | 26.085 | 36.067 | 77.738 | 1.00 68.93 | AAAA |
| MOTA | 2267 | - | . GLU | 284 | 27.198 | 37.133 | 79.309 | 1.00 72.01 | AAAA |
| MOTA | 2268 | OE2 | | 284 | | 31.862 | 77.733 | 1.00 31.57 | AAAA |
| MOTA | 2269 | С | GLU | 284 | 29.181 | 31.310 | 78.803 | 1.00 33.08 | AAAA |
| MOTA | 2270 | 0 | GLU | 284 | 29.410 | | 76.686 | 1.00 23.37 | AAAA |
| MOTA | 2271 | N | VAL | 285 | 28.673 | 31.221 | 76.774 | 1.00 23.25 | AAAA |
| ATOM | 2272 | CA | VAL | 285 | 28.354 | 29.807 | | 1.00 23.23 | AAAA |
| ATOM | 2273 | CB | VAL | 285 | 27.221 | 29.407 | 75.789 | 1.00 26.98 | AAAA |
| ATOM | 2274 | CG1 | VAL | 285 | 26.952 | 27.913 | 75.881 | 1.00 20.90 | AAAA |
| ATOM | 2275 | | VAL | 285 | 25.940 | 30.181 | 76.107 | 1.00 24.98 | AAAA |
| | 2276 | Ċ. | | 285 | 29.567 | 28.942 | 76.479 | 1.00 31.41 | |
| MOTA | | ò | VAL | 285 | 29.833 | 27.983 | 77.195 | 1.00 25.34 | AAAA |
| MOTA | 2277 | | PHE | 286 | 30.316 | 29.276 | . 75.431 | 1.00 27.27 | AAAA |
| MOTA | 2278 | N | | 286 | 31.463 | 28.457 | 75.086 | 1.00 22.47 | AAAA |
| MOTA | 2279 | CA | PHE | 286 | 31.289 | 27.904 | 73.667 | 1.00 22.26 | AAAA |
| MOTA | 2280 | CB | PHE | | 30.168 | 26.918 | 73.536 | 1.00 25.71 | AAAA |
| MOTA | 2281 | CG | PHE | 286 | 28.971 | 27.274 | 72.917 | 1.00 22.88 | AAAA |
| MOTA | 2282 | | 1 PHE | 286 | 30.294 | 25.631 | 74.069 | 1.00 24.49 | AAAA |
| MOTA | 2283 | | 2 PHE | 286 | | 26.365 | 72.829 | 1.00 19.85 | AAAA |
| ATOM | . 2284 | | 1 PHE | 286 | 27.919 | 24.714 | 73.987 | 1.00 27.48 | AAAA |
| ATOM | 2285 | CE: | 2 PHE | 286 | 29.246 | | | 1.00 24.59 | AAAA |
| ATOM | 2286 | CZ | PHE | 286 | 28.056 | 25.081 | | 1.00 21.53 | AAAA |
| ATOM | 2287 | С | PHE | 286 | 32.854 | 29.059 | | 1.00 27.12 | AAAA |
| ATOM | 2288 | 0 | PHE | 286 | 33.849 | 28.417 | 74.873 | 1.00 27.12 | AAAA |
| MOTA | 2289 | N | GLY | 287 | 32.937 | | 75.754 | 1.00 23.70 | AAAA |
| | 2290 | CA | | 287 | 34.237 | | 75 901 | 1.00 24.17 | AAAA |
| ATOM | 2291 | C | GLY | 287 | 34.705 | 31.419 | 74.562 | 1.00 27.05 | • |
| ATOM | 2292 | ō | GLY | 287 | 33.888 | 31.670 | • 73.667 | 1.00 18.06 | AAAA |
| MOTA | | | GLU | 288 | 36.017 | 31.576 | 74.414 | 1.00 23.21 | AAAA |
| MOTA | 2293 | N | | 288 | 36.583 | | 73.170 | 1.00 24.87 | AAAA |
| MOTA | 2294 | CA | | 288 | 37.968 | | | 1.00 29.25 | AAAA |
| MOTA | 2295 | CB | | | 37.984 | | | 1.00 42.63 | AAAA |
| MOTA | 2296 | CG | | 288 | 37.114 | | | 1.00 43.77 | AAAA |
| ATOM | 2297 | CD | | 288 | 37.235 | | | | AAAA |
| ATOM | 2298 | | 1 GLU | 288 | | | | | AAAA |
| MOTA | 2299 | OE | 2 GLU | 288 | 36.317 | | | | AAAA |
| ATOM | 2300 | С | GLU | 288 | 36.693 | | | | AAAA |
| ATOM | 2301 | | GLU | 288 | 36.995 | | | | AAAA |
| MOTA | 2302 | | GLY | 289 | 36.447 | | | | AAAA |
| ATOM | 2303 | | | 289 | 36.517 | | | | AAAA |
| | 2304 | | GLY | 289 | 37.126 | 31.318 | | | AAAA |
| ATOM | 2305 | | GLY | 289 | 37.669 | 32.404 | | 1.00 16.59 | AAAA |
| ATOM | | | VAL | 290 | 37.032 | | 4 67.322 | | |
| MOTA | 2306 | | | 290 | 37.572 | | | 1.00 19.70 | AAAA |
| MOTA | | | | | 38.150 | | | 1 1.00 19.04 | AAAA |
| MOTA | | CE | | 290 | 38.66 | | | 1.00 15.54 | AAAA |
| MOTA | 2309 | | 1 VAL | 290 | 30.00 | | | | AAAA |
| MOTA | |) CG | 2 VAL | 290 | 39.29 | , 69,40. | | | |

| | | _ | *** * | 290 | 36.408 | 32.040 | 65.427 | 1.00 20.90 | AAAA |
|------|--------------|-----------|------------|-------------|--------|--------|--------|------------|------|
| MOTA | 2311 | _ | VAL | | 35.351 | 31.439 | 65.193 | 1.00 19.33 | AAAA |
| MOTA | 2312 | | VAL | 290 | 36.598 | 33.325 | 65.125 | 1.00 15.37 | AAAA |
| ATOM | 2313 | N | TYR | 291 | _ | 34.140 | 64.524 | 1.00 16.79 | AAAA |
| MOTA | 2314 | CA | TYR | 291 | 35.543 | 35.438 | 65.317 | 1.00 16.42 | AAAA |
| MOTA | 2315 | CB | TYR | 291 | 35.412 | 35.181 | 66.808 | 1.00 18.60 | AAAA |
| ATOM | 2316 | CG | TYR | 291 | 35.375 | | 67.659 | 1.00 21.77 | AAAA |
| ATOM | 2317 | CD1 | TYR | 291 | 36.366 | 35.688 | | 1.00 22.55 | AAAA |
| MOTA | 2318 | CE1 | TYR | 291 | 36.368 | 35.385 | 69.030 | 1.00 22.33 | AAAA |
| ATOM | 2319 | CD2 | TYR | . 291 | 34.388 | 34.374 | 67.361 | 1.00 20.24 | AAAA |
| ATOM | 2320 | CE2 | TYR | 291 | 34.381 | 34.066 | 68.718 | 1.00 25.85 | AAAA |
| ATOM | 2321 | CZ | TYR | 291 - | 35.367 | 34.568 | 69.545 | 1.00 25.57 | AAAA |
| ATOM | 2322 | OH | TYR | 291 | 35.338 | 34.246 | 70.885 | 1.00 23.37 | AAAA |
| ATOM | 2323 | С | TYR | 291 | 35.720 | 34.446 | 63.031 | | AAAA |
| ATOM | 2324 | 0 | TYR | 291 | 36.773 | 34.921 | 62.586 | 1.00 15.21 | AAAA |
| ATOM | 2325 | N | LEU | 292 | 34.660 | 34.189 | 62.273 | 1.00 14.06 | AAAA |
| MOTA | 2326 | CA | LEU | 292 | 34.674 | 34.392 | 60.824 | 1.00 15.03 | AAAA |
| ATOM | 2327 | CB | LEU | 292 | 34.461 | 33.046 | 60.108 | 1.00 13.66 | AAAA |
| ATOM | 2328 | CG | LEU | 292 | 35.342 | 31.856 | 60.496 | 1.00 19.04 | AAAA |
| MOTA | 2329 | | LEU | 292 | 34.909 | 30.615 | 59.665 | 1.00 15.17 | |
| ATOM | 2330 | | LEU | 292 | 36.792 | 32.190 | 60.252 | 1.00 19.18 | AAAA |
| ATOM | 2331 | C | LEU | 292 | 33.564 | 35.327 | 60.396 | 1.00 16.62 | AAAA |
| | 2332 | ō | LEU | 292 | 32.575 | 35.488 | 61.107 | 1.00 14.76 | AAAA |
| ATOM | 2332 | N | GLY | 293 | 33.724 | 35.932 | 59.216 | 1.00 18.62 | AAAA |
| MOTA | 2334 | CA | GLY | 293 | 32.696 | 36.816 | 58.699 | 1.00 17.10 | AAAA |
| MOTA | 2335 | C | GLY | 293 | 31.611 | 35.954 | 58.068 | 1.00 23.44 | AAAA |
| MOTA | | 0 | GLY | 293 | 31.407 | 34.798 | 58.459 | 1.00 23.60 | AAAA |
| MOTA | 2336 2337 | N | GLY | 294 | 30.915 | 36.501 | 57.085 | 1.00 24.96 | AAAA |
| ATOM | | CA | GLY | 294 | 29.871 | 35.738 | 56.434 | 1.00 27.07 | AAAA |
| MOTA | 2338 | C | GLY | 294 | 29.132 | 36.632 | 55.474 | 1.00 28.41 | AAAA |
| MOTA | 2339 | 0 | GLY | 294 | 29.605 | 37.722 | 55.167 | 1.00 25.66 | AAAA |
| ATOM | 2340 | | GLY | 295 | 27.972 | 36.168 | 55.011 | 1.00 20.33 | AAAA |
| ATOM | 2341 | N | GLY | 295 | 27.164 | 36.936 | 54.085 | 1.00 20.14 | AAAA |
| MOTA | 2342 | CA C | GLY | 295 | 26.742 | 38.244 | 54.730 | 1.00 25.34 | AAAA |
| MOTA | 2343 | | GLY | 295 | 26.550 | 38.317 | 55.942 | 1.00 28.89 | AAAA |
| MOTA | 2344 | .0 | GLY | 296 | 26.614 | 39.274 | 53.909 | 1.00 28.52 | AAAA |
| MOTA | 2345 | N | GLY | 296 | 26.230 | 40.598 | 54.367 | 1.00 23.21 | AAAA |
| MOTA | .2346 | CA | GLY | 296 | 26.314 | 41.342 | 53.059 | 1.00 26.34 | AAAA |
| MOTA | 2347 | C | GLY | 296 | 27.359 | 41.324 | 52.414 | 1.00 26.05 | AAAA |
| ATOM | 2348 | 0 | TYR | 297 | 25.235 | 42.008 | 52.662 | 1.00 22.61 | AAAA |
| ATOM | 2349 | N | TYR | 297 | 25.228 | 42.644 | 51.360 | 1.00 22.58 | AAAA |
| MOTA | 2350 | CA | TYR | 297 | 24.265 | 41.861 | 50.457 | 1.00 23.68 | AAAA |
| ATOM | 2351 | CB | TYR | 297 | 24.502 | 40.352 | 50.521 | 1.00 25.14 | AAAA |
| ATOM | 2352 | CG CD1 | | 297 | 23.981 | 39.571 | 51.568 | 1.00 28.31 | AAAA |
| MOTA | 2353 | CE1 | | 297 | 24.269 | 38.196 | 51.662 | 1.00 24.18 | AAAA |
| ATOM | 2354 | | | 297 | 25.307 | 39.725 | 49.577 | 1.00 29.74 | AAAA |
| MOTA | 2355 | CD2 | | 297 | 25.598 | 38.362 | 49.664 | 1.00 27.09 | AAAA |
| ATOM | 2: 36 | | | 297 | 25.085 | 37.606 | 50.696 | 1.00 28.68 | AAAA |
| ATOM | 257 | CZ | TYR TYR | 297 | 25.407 | 36.261 | 50.739 | 1.00 28.17 | AAAA |
| MOTA | 2538 | ОН | TYR | 297 | 24.916 | 44.138 | 51.320 | 1.00 24.98 | AAAA |
| ATOM | 2359 | C | | 297 | 24.841 | 44.714 | 50.237 | 1.00 26.51 | AAAA |
| ATOM | 2360 | 0 | TYR | 298 | 24.740 | 44.752 | 52.491 | 1.00 23.80 | AAAA |
| ATOM | 2361 | N | HIS | 298 | 24.480 | 46.188 | 52.591 | 1.00 23.44 | AAAA |
| ATOM | 2362 | CY | HIS | 298. | 23.325 | | | 1.00 23.37 | AAAA |
| MOTA | 2363 | CB | HIS | 298. 298 | 22.956 | | | 1.00 32.94 | AAAA |
| ATOM | 2364 | CG | HIS | | 23.491 | | | 1.00 24.31 | AAAA |
| MOTA | 2365 | | HIS | 298 | 22.011 | | | 1.00 38.29 | AAAA |
| MOTA | 2366 | | HIS | 298 | 21.978 | | | 1.00 25.60 | AAAA |
| MOTA | 2367 | | HIS | 298 | 22.867 | | 53.788 | 1.00 36.57 | AAAA |
| ATOM | 2368 | | 2 HIS | 298 | 25.757 | | | 1.00 23.11 | AAAA |
| MOTA | 2369 | C | HIS | 298 | 26.135 | 46.439 | | 1.00 22.64 | AAAA |
| ATOM | 2370 | 0 | HIS | 298 | 26.430 | | _ | 1.00 21.07 | АААА |
| ATOM | 2371 | N | PRO | 399 | 26.078 | | | 1.00 27.42 | AAAA |
| ATOM | 2372 | CD | | 299 | 27.676 | | | | AAAA |
| ATOM | 2373 | | | 299 | 28.041 | | | 1.00 28.95 | AAAA |
| ATOM | 2374 | | | 299 | 26.678 | | | 1.00 35.16 | AAAA |
| ATOM | 2375 | | | 299 | | | | | AAAA |
| ATOM | 2376 | С | PRO | 299 | 27.049 | | | | • |
| •• | | | | • | | | | | |

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| | | | | | 28.565 | 48.845 | 55.068 | 1.00 24.36 | AAAA |
|--------|-------|-------|--------------|-------------|------------------|----------|----------|--------------|------|
| MOTA | 2377 | | PRO | 299 | 26.602 | 49.769 | | 1.00 24.48 | AAAA |
| ATOM | 2378 | _ | ryr | 300 | | 50.478 | | 1.00 22.94 | AAAA |
| ATOM | 2379 | - | TYR | 300 | 26.495 | 51.442 | | 1.00 25.24 | AAAA |
| ATOM | 2380 | | TYR | 300 | 25.317 | 52.599 | | 1.00 30.44 | AAAA |
| ATOM | 2381 | | TYR | 300 | 25.411 | 52.634 | 53.746 | 1.00 26.01 | AAAA |
| ATOM | 2382 | CD1 ' | TYR | 300 | 26.366 | 53.676 | | 1.00 29.66 | AAAA |
| ATOM | 2383 | CE1 ' | TYR | 300 | 26.389 | 53.640 | 54.827 | 1.00 31.37 | AAAA |
| MOTA | 2384 | CD2 | TYR | 300 | 24.490 | | 53.916 | 1.00 35.88 | AAAA |
| MOTA | 2385 | CE2 | TYR | 300 | 24.501 | 54.677 | 52.913 | 1.00 38.44 | AAAA |
| ATOM | 2386 | CZ - | TYR | 300 | 25.448 | 54.689 | 51.990 | 1.00 33.41 | AAAA |
| ATOM | 2387 | OH | TYR | 300 | 25.417 | 55.700 | 56.921 | 1.00 22.80 | AAAA |
| MOTA | 2388 | ·C | TYR . | 300 | 26.280 | 49.515 | 57.983 | 1.00 19.14 | AAAA |
| ATOM | 2389 | 0 | TYR | 300 . | 26.895 | 49.643 | 56.705 | 1.00 23.08 | AAAA |
| MOTA | 2390 | N | ALA | 301 | 25.374 | 48.568 | 57.719 | 1.00 21.68 | AAAA |
| ATOM | 2391 | CA | ALA | 301 | 25.009 | 47.589 | 57.198 | 1.00 19.52 | AAAA |
| ATOM | 2392 | CB | ALA | 301 | 23.893 | 46.687 | 58.098 | 1.00 23.49 | AAAA |
| ATOM | 2393 | С | ALA | 301 | 26.216 | 46.762 | 59.274 | 1.00 21.21 | AAAA |
| ATOM | 2394 | | ALA | 301 | 26.507 | 46.570 | 57.072 | 1.00 23.19 | AAAA |
| ATOM | 2395 | | LEU | 302 | 26.904 | 46.275 | | 1.00 20.66 | AAAA |
| ATOM | 2396 | CA | LEU | 302 | 28.090 | 45.463 | 57.234 | 1.00 23.31 | AAAA |
| | 2397 | CB | LEU | 302 | 28.602 | 45.057 | 55.844 | 1.00 36.66 | AAAA |
| MOTA | 2398 | ĊĞ | LEU ' | 302 | 29.932 | 44.335 | 55.611 | 1.00 38.41 | AAAA |
| MOTA | 2399 | CD1 | | 302 | 29.979 | 43.849 | 54.170 | | AAAA |
| ATOM | _ | | LEU | 302 | 31.104 | 45.255 | 55.879 | 1.00 28.52 | AAAA |
| MOTA | 2400 | | LEU | 302 | 29.165 | 46.204 | 58.012 | 1.00 22.08 | AAAA |
| MOTA | 2401 | С | LEU | 302 | 29.653 | 45.713 | 59.020 | 1.00 20.43 | |
| MOTA | 2402 | 0 | ALA | 303 | 29.517 | 47.401 | 57.549 | 1.00 19.58 | AAAA |
| MOTA | 2403 | N | ALA | 303 | 30.567 | 48.173 | 58.197 | 1.00 19.77 | AAAA |
| MOTA | 2404 | CA | | 303 | 30.816 | 49.460 | 57.432 | 1.00 21.69 | AAAA |
| MOTA | 2405 | · CB | ALA | 303 | 30.324 | 48.485 | 59.657 | 1.00 19.19 | AAAA |
| MOTA | 2406 | C | ALA | 303 | 31.216 | 48.310 | 60.489 | 1.00 22.51 | AAAA |
| MOTA | 2407 | 0 | ALA | 304 | 29.128 | 48.954 | 59.993 | 1.00 20.12 | AAAA |
| MOTA | 2408 | N | ARG | 304 | 28.872 | | 61.377 | 1.00 18.04 | AAAA |
| MOTA . | 2409 | CA | ARG | 304 · | 27.566 | | 61.511 | 1.00 21.09 | AAAA |
| ATOM | 2410 | CB | ARG | 304 | 27.532 | | 60.792 | 1.00 24.34 | AAAA |
| MOTA | 2411 | CG | ARG | | 26.259 | | 61.206 | 1.00 27.09 | AAAA |
| MOTA | 2412 | CD | ARG | 304 | 25.090 | | 61.116 | 1.00 45.73 | AAAA |
| MOTA | 2413 | NE | ARG | 304 | 23.965 | | 61.808 | 1.00 39.82 | AAAA |
| ATOM | 2414 | CZ | ARG | 304 | 23.813 | | 62.677 | 1.00 28.40 | AAAA |
| MOTA | 2415 | NH1 | | 304 | 22.991 | | 61.647 | 1.00 41.77 | AAAA |
| MOTA | 2416 | | ARG | 304 | 28.794 | | | 1.00 21.00 | AAAA |
| MOTA | 2417 | С | ARG | 304 | 29.313 | | | 1.00 19.45 | AAAA |
| MOTA | 2418 | 0 | ARG | 304 | 29.313 | | | 1.00 19.93 | AAAA |
| MOTA | 2419 | N | ALA | 305 | 28.159 28.002 | | | 1.00 18.70 | AAAA |
| ATOM | 2420 | CA | λ LA | 305 | | | | 1.00 18.26 | AAAA |
| ATOM | 2421 | CB | ALA | 305 | 26.998 | | | 1.00 16.46 | AAAA |
| ATOM | 2422 | С | ALA | 3 05 | 29.311 | | | 1.00 .9.49 | AAAA |
| MOTA | 2423 | 0 | ALA | 305 | 29.564 | | | | AAAA |
| MOTA | 2424 | N | TRP | 306 | 30.15 | | | | AAAA |
| MOTA | 2425 | CA | TRP | 306 | 31.42 | _ | | | AAAA |
| MOTA | 2426 | | TRP | 306 | 32.15 | 1 43.865 | | | AAAA |
| ATOM | 2427 | | TRP | 306 | 31.63 | | | | AAAA |
| ATOM | 2428 | | 2 TRP | 306 | 31.85 | | | | AAAA |
| ATOM | 2429 | | 2 TRP | 306 | 31.24 | | | | AAAA |
| ATOM | 2430 | | 3 TRP | 306 | 32.50 | | 57.878 | | AAAA |
| ATOM | | | 1 TRP | 306 | 30.91 | | 60.995 | | AAAA |
| | | | | 306 | 30.68 | | | | AAAA |
| MOTA | | | | 306 | 31.27 | 0 40.00 | | | AAAA |
| MOTA | | | _ | 306 | 32.53 | | | | AAAA |
| ATOM | | - | | 306 | 31.91 | 7 40.51 | | | AAAA |
| ATOM | | | TRP | 306 | 32.28 | 9 45.18 | 8 63.018 | | AAAA |
| ATOM | | | | 306 | 33.15 | | 6 63.752 | | |
| ATOM | | | TRP | 307 | .32.06 | | 1 62.913 | | AAAA |
| ATOM | | | THR | 307 | 32.84 | | 2 63.72 | | AAAA |
| ATOM | 2439 | | | 307 | 32.57 | | 5 63.31 | | AAAA |
| ATOM | | _ | | | 33.21 | | | 1 1.00 21.58 | AAAA |
| ATOM | 1 044 | | 1 THR | 307 | 33.12 | | | | AAAA |
| ATOM | | 2 CG | 2 THR | 307 | ٠. ٠. ١ | | • | | • |
| | • | | • | | | | | | |

| | | | | | _ | | | | |
|--------------|--------------|-----------|------------|------------|------------------|------------------|------------------|--------------------------|------------------|
| | | | | 207 | 32.493 | 47.146 | 65.187 | 1.00 17.47 | AAAA |
| MOTA | 2443 | C | THR | 307 307 | 33.377 | 47.142 | 66.039 | 1.00 18.94 | AAAA |
| ATOM | 2444 | 0 | THR | 307 | 31.216 | 46.901 | 65.487 | 1.00 19.97 | AAAA |
| MOTA | 2445 | | LEU | 308 | 30.834 | 46.587 | 66.866 | 1.00 22.54 | AAAA |
| MOTA | 2446 | | LEU | 308 | 29.318 | 46.365 | 66.989 | 1.00 21.13 | AAAA |
| MOTA | 2447 | | LEU LEU | 308 | 28.415 | 47.579 | 66.751 | 1.00 22.82 | AAAA |
| ATOM | 2448 | CG CD1 | | 308 | 26.937 | 47.219 | 67.023 | 1.00 25.01 | AAAA |
| MOTA | 2449 | CD2 | | 308 | 28.870 | 48.710 | 67.685 | 1.00 29.09 | AAAA |
| MOTA | 2450 2451 | CDZ | LEU | 308 | 31.578 | 45.331 | 67.336 | 1.00 22.98 | AAAA |
| MOTA | 2452 | 0 | LEU | 308 | 32.056 | 45.250 | 68.479 | 1.00 22.27 | AAAA |
| ATOM ATOM | 2453 | N | ILE | 309 | 31.677 | 44.342 | 66.454 | 1.00 22.54 | AAAA AAAA |
| ATOM | 2454 | CA | ILE | 309 | 32.377 | 43.114 | 66.801 | 1.00 17.09 | AAAA |
| ATOM | 2455 | CB | ILE | 309 | 32.318 | 42.073 | 65.664 | 1.00 18.12 1.00 24.16 | AAAA |
| ATOM | 2456 | CG2 | | 309 | 33.170 | 40.870 | 66.033 | 1.00 24.16 | AAAA |
| ATOM | 2457 | CG1 | | 309 | 30.871 | 41.655 | 65.399 | 1.00 18.23 | AAAA |
| MOTA | 2458 | CD1 | | 309 | 30.205 | 40.989 | 66.586 67.067 | 1.00 20.84 | AAAA |
| ATOM | 2459 | С | ILE | 309 | 33.849 | 43.410 | 68.031 | 1.00 25.20 | AAAA |
| MOTA | 2460 | 0 | ILE | 309 | 34.426 | 42.905 | 66.214 | 1.00 16.86 | AAAA |
| ATOM | 2461 | N | TRP | 310 | 34.466 | 44.223 44.517 | 66.411 | 1.00 17.86 | AAAA |
| MOTA | 2462 | CA | TRP | 310 | 35.888 36.439 | 45.319 | 65.235 | 1.00 14.83 | AAAA |
| MOTA | 2463 | СВ | TRP | 310 | 37.879 | 45.648 | 65.397 | 1.00 16.63 | AAAA |
| MOTA | 2464 | CG | TRP | 310 | 38.967 | 44.718 | 65.560 | 1.00 18.62 | AAAA |
| MOTA | 2465 | CD2 | TRP | 310 | 40.131 | 45.478 | 65.799 | 1.00 25.60 | AAAA |
| MOTA | 2466 | CE2 | TRP | 310 310 | 39.069 | 43.319 | 65.529 | 1.00 24.06 | AAAA |
| MOTA | 2467 | CE3 | TRP TRP | 310 | 38.418 | 46.895 | 65.533 | 1.00 19.82 | AAAA |
| MOTA | 2468 2469 | | TRP | 310 | 39.768 | 46.801 | 65.777 | 1.00 25.84 | AAAA |
| MOTA | 2470 | CZ2 | | 310 | 41.383 | 44.887 | 66.006 | 1.00 26.14 | AAAA |
| MOTA MOTA | 2471 | CZ3 | TRP | 310 | 40.308 | 42.730 | 65.735 | 1.00 24.89 | AAAA AAAA |
| ATOM | 2472 | | TRP | 310 | 41.452 | 43.515 | 65.971 | 1.00 24.96 1.00 20.86 | AAAA |
| ATOM | 2473 | C | TRP | 310 | 36.112 | 45.263 | 67.733 | 1.00 20.88 | AAAA |
| ATOM | 2474 | 0 | TRP | 310 | 37.050 | 44.957 | 68.478 | 1.00 24.22 | AAAA |
| ATOM | 2475 | N | CYS | 311 | 35.242 | 46.226 | 68.030 69.280 | 1.00 27.66 | AAAA |
| ATOM | 2476 | CA | CYS | 311 | 35.349 | 46.971 | 69.343 | 1.00 25.37 | AAAA |
| ATOM | 2477 | CB | CYS | 311 | 34.297 | 48.097 49.528 | 68.253 | 1.00 27.22 | AAAA |
| MOTA | 2478 | SG | CYS | 311 | 34.618 35.224 | 46.042 | 70.490 | 1.00 22.95 | AAAA |
| MOTA | 2479 | C | CYS | 311 | 35.986 | 46.180 | 71.441 | 1.00 25.47 | AAAA |
| MOTA | 2480 | 0 | CYS | 311 312 | 34.284 | 45.089 | 70.457 | 1.00 17.03 | AAAA |
| ATOM | 2481 | N | GLU | 312 | 34.120 | 44.129 | 71.569 | 1.00 22.44 | AAAA |
| MOTA | 2482 | CA | GLU GLU | 312 | 33.011 | 43.110 | 71.280 | 1.00 20.81 | AAAA |
| MOTA | 2483 2484 | CB CG | GLU | 312 | 31.856 | 43.048 | 72.258 | 1.00 43.65 | AAAA |
| ATOM | 2485 | CD | GLU | 312 | 32.265 | 42.971 | 73.717 | 1.00 29.63 | AAAA AAAA |
| ATOM ATOM | 2486 | | GLU | 312 | 33.022 | | 74.119 | 1.00 38.85 1.00 53.22 | AAAA |
| ATOM | 2487 | OE2 | | 312 | 31.804 | | 74.473 | 1.00 53.22 | AAAA |
| ATOM | 2488 | c | GLI | 312 | 35.395 | 43.309 | 71.778 | 1.00 27.47 | AAAA |
| ATOM | 2489 | Ō | GLì. | 312 | 35.899 | | | 1.00 23.82 | AAAA |
| ATOM | 2490 | N | LEL | 313 | 35.899 | | | 1.00 20.72 | AAAA |
| MOTA | 2491 | CA | LEU | 313 | 37.101 | 41.889 | | 1.00 27.82 | AAAA |
| ATOM | 2492 | CB | LEU | 313 | 37.380 | | | 1.00 33.55 | AAAA |
| MOTA | 2493 | CG | LEU | 313 | 36.403 | | | 1.00 24.03 | AAAA |
| MOTA | 2494 | | LEU | 313 | 36.839 36.379 | | | | AAAA |
| ATOM | 2495 | | LEU | 313 | 38.343 | | * | | AAAA |
| MOTA | 2496 | | LEU | 313 | 39.119 | | | 1.00 21.48 | AAAA |
| ATOM | 2497 | | LEU | 313 | 38.492 | | | 1.00 19.41 | AAAA |
| MOTA | 2498 | | SER | 314 | 39.627 | | | 1.00 28.26 | AAAA |
| MOTA | 2499 | | SER | 314 314 | 39.625 | | | 1.00 22.55 | AAAA |
| ATOM | 2500 | | SER | 314 | 40.732 | | 69.759 | 1.00 61.92 | AAAA |
| ATOM | 2501 | | | 314 | 39.619 | | | 1.00 30.18 | AAAA |
| MOTA | 2502 | | SER SER | 314 | 40.63 | | 72.590 | | AAAA |
| ATOM | 2503 | | GLY | 315 | 38.47 | | 72.806 | | AAAA AAAA |
| MOTA | 2504 2505 | | | 315 | 38.39 | 3 46.009 | | | AAAA |
| MOTA | 2506 | | GLY | | 38.32 | 4 47.518 | | 1.00 36.93 | AAAA |
| ATOM | 2507 | | GLY | | 38.81 | 1 48.178 | | | AAAA. |
| ATOM | | i N | ARG | | 37.73 | 9 48.090 | 73.065 | 1.00 31.33 | , And the second |

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Figure 16-39

| | | | | | | | | 73 043 | 1.00 39.10 | AAAA |
|-----|---------|------|-----|-------|-----|------------------|--------------------|---------------|--------------|----------------|
| _ | | 2509 | CA | ARG | 316 | 37.631 | 49.536 | | | |
| | TOM | | | | 316 | 38.347 | 50.108 | 71.830 | 1.00 45.15 | AAAA |
| A | TOM | 2510 | CB | ARG | | | | 70.501 | 1.00 46.02 | AAAA |
| | TOM | 2511 | CG | ARG | 316 | 37.722 | | | 1.00 44.83 | AAAA |
| | | 2512 | CD | ARG | 316 | 38.620 | 50.45 9 | 69.449 | | |
| A | MOT | | | | 316 | 39.898 | 49.767 | 69.357 | 1.00 37.91 | AAAA |
| A | MOT. | 2513 | NE | ARG | | | _ | 68.674 | 1.00 27.39 | AAAA |
| | TOM | 2514 | CZ | ARG | 316 | 40.945 | | | | AAAA |
| | | | NHl | | 316 | 40.854 | 51.371 | 68.034 | 1.00 50.24 | |
| A | TOM | 2515 | | | | | | 68.572 | 1.00 34.51 | AAAA |
| 2 | MOT | 2516 | NH2 | ARG | 316 | 42.054 | | | 1.00 35.43 | AAAA |
| | | 2517 | С | ARG | 316 | 36.179 | 49.984 | 73.058 | 1.00 33.43 | |
| | MOT | | | | 316 | 35.292 | 49.271 | 72.596 | 1.00 30.71 | AAAA |
| 7 | MOT | 2518 | 0 | ARG | | | | 73.612 | 1.00 34.06 | AAAA |
| | MOTA | 2519 | N | GLU | 317 | 35.93 | | | 1.00 37.96 | AAAA |
| | | _ | CA | GLU | 317 | 34.569 | 51.663 | 73.671 | | |
| 7 | MOTA | 2520 | | | | 34.48 | | 74.552 | 1.00 43.60 | AAAA |
| 7 | MOTA | 2521 | CB | GLU | 317 | | | 75.960 | 1.00 60.36 | AAAA |
| | MOTA | 2522 | CG | GLU | 317 | 33.96 | | | 1.00 00.30 | AAAA |
| | | - | | GLU | 317 | 34.76 | 8 51.575 | 76.701 | 1.00 70.70 | |
| - 2 | MOTA | 2523 | CD | | | 34.37 | | 77.832 | 1.00 76.71 | AAAA |
| | MOTA | 2524 | OE1 | GLU | 317 | | | | 1.00 78.36 | AAAA |
| | | 2525 | OE2 | GLU | 317 | 35.79 | | 76.162 | | AAAA |
| | MOTA | 2323 | | GLU | 317 | 34.06 | 8 51.958 | 72.280 | 1.00 35.65 | |
| - 1 | MOTA | 2526 | С | | | | | 71.390 | 1.00 32.91 | AAAA |
| : | MOTA | 2527 | 0 | GLU | 317 | 34.84 | | | 1.00 30.52 | AAAA |
| | | 2528 | N | VAL | 318 | 32.76 | 7 51.772 | 72.094 | | AAAA |
| | MOTA | | | | 318 | 32.13 | | 70.808 | 1.00 37.04 | |
| | MOTA | 2529 | ÇA | VAL | | | | 70.638 | 1.00 36.48 | AAAA |
| | MOTA | 2530 | CB | VAL | 318 | 30.87 | | | 1.00 40.43 | AAAA |
| | | | | VAL | 318 | 30.27 | 8 51.366 | 69.268 | | |
| | MOTA | 2531 | | | | 31.22 | | 70.846 | 1.00 33.75 | AAAA |
| | MOTA | 2532 | CG2 | VAL | 318 | | | 70.737 | 1.00 28.96 | AAAA |
| | MOTA | 2533 | С | VAL | 318 | 31.71 | 9 53.465 | | 1.00 33.56 | AAAA |
| | | | ō | VAL | 318 | 30.93 | 0 53.915 | 71.556 | 1.00 33.50 | |
| | MOTA | 2534 | | | | 32.25 | | 69.773 | 1.00 29.20 | AAAA |
| | MOTA | 2535 | N | PRO | 319 | | | 68.726 | 1.00 31.62 | AAAA |
| | ATOM | 2536 | CD | PRO | 319 | 33.24 | | | 1.00 28.99 | AAAA |
| | | | CA | PRO | 319 | 31.85 | 8 55.637 | | | |
| | MOTA | 2537 | | | | 32.70 | | 68.528 | 1.00 32.17 | AAAA |
| | ATOM | 2538 | CB | PRO | 319 | 52.70 | | | 1.00 41.36 | AAAA |
| | ATOM | 2539 | CG | PRO | 319 | 32.85 | 0 54.926 | | 1.00 36.95 | AAAA |
| | | | | PRO | 319 | 30.36 | 5 55.680 | 69.377 | | |
| | MOTA | 2540 | С | | | 29.84 | | 68.695 | 1.00 32.86 | AAAA |
| | ATOM | 2541 | 0 | PRO | 319 | | | | 1.00 34.61 | AAAA |
| | ATOM | 2542 | · N | GLU | 320 | 29.64 | 6 56.683 | | 1 00 35 13 | AAAA |
| | | | | GLU | 320 | 28.23 | 0 56.657 | 69.544 | 1.00 35.13 | |
| | MOTA | 2543 | CA | | | 27.41 | 9 57.416 | 70.595 | 1.00 52.97 | AAAA |
| | ATOM | 2544 | CB | GLU | 320 | | ., ., | 70.738 | 1.00 56.06 | AAAA |
| | | 2545 | CG | GLU | 320 | 27.75 | 58.875 | 70.730 | | AAAA |
| | MOTA | | | GLU | 320 | 26.82 | 22 59.558 | 71.721 | 1.00 65.58 | |
| | MOTA | 2546 | CD | | | 25.60 | | | 1.00 64.27 | AAAA |
| | MOTA | 2547 | OE: | L GLU | 320 | 25.00 | | | 1.00 72.99 | AAAA |
| | | 2548 | OES | 2 GLU | 320 | 27.30 | | | 1.00 72.33 | AAAA |
| | MOTA | | | | 320 | 27.94 | 13 57.192 | 68.153 | 1.00 35.13 | |
| | MOTA | 2549 | С | GLU | | 26.9 | | 67.565 | 1.00 37.43 | AAAA |
| | MOTA | 2550 | 0 | GLU | 320 | | - : | | 1.00 28.22 | AAAA |
| | | 2551 | N | LYS | 321 | 28.8 | 30 57.953 | | 1.00 20.22 | AAAA |
| | ATOM | | | | 321 | 28.7 | 00 58.55 | 66.289 | 1.00 36.58 | |
| | ATOM | 2552 | CA | | | 28.6 | | | 1.00 44.87 | AAAA |
| | ATOM | 2553 | CB | LYS | 321 | 28.0 | | | 1.00 55.73 | . ` AAA |
| | | 2554 | CG | LYS | 321 | 29.9 | 87 60.60 | | 1.00 55.75 | AAA |
| | ATOM | | | | 321 | 30.3 | | 68.410 | 1.00 57.27 | |
| | ATOM | 2555 | CD | LYS | | | | 0 68.840 | 1.00 54.59 | AAA |
| | MOTA | 2556 | CE | LYS | 321 | 31.7 | | | | AAAA |
| | | 2557 | NZ | LYS | 321 | 32.0 | 24 61.77 | | | AAAA |
| | MOTA | 2337 | 112 | | | 29.8 | | 1 65.315 | | |
| | ATOM | 2558 | С | LYS | 321 | | | | 1.00 33.83 | AAAA |
| | ATOM | 2559 | 0 | LYS | 321 | 30.9 | | | | AAAA |
| | | 2560 | | LEU | 322 | 29.5 | 49 58.35 | | | AAAA |
| | MOTA | | | | | 30.5 | | 5 62.998 | 1.00 29.45 | |
| | MOTA | 2561 | CA | | 322 | | | | | AAAA |
| | ATOM | 2562 | СВ | LEU | 322 | 29.9 | | | | AAAA |
| | | | | | 322 | 29.2 | 40 56.33 | 8 61.651 | | |
| | ATOM | 2563 | | | | 29.0 | 08 55.97 | 7 60.186 | 1.00 38.44 | aaaj |
| | MOTA | 2564 | CD | 1 LEU | 322 | | | | | LAAA |
| | | 2565 | | 2 LEU | 322 | 30.0 | 72 55.26 | | | AAA |
| | ATOM | | | | 322 | 31.2 | 28 59.50 | 3 62.783 | 1.00 33.28 | |
| | MOTA | 2566 | | LEU | | 30.5 | | | 1.00 31.45 | AAA |
| | ATOM | 2567 | 0 | LEU | 322 | 30.2 | | | | AAAi |
| | | 2568 | | ASN | 323 | 32.5 | 33 59.53 | | | AAA |
| | ATOM | | | | | 33.2 | | 4 62.294 | | |
| | ATOM | 2569 | CA | | | 22.2 | | | | AAA |
| | ATOM | 2570 | CE | 3 ASN | 323 | 34.7 | | | | AAA. |
| | | | | | | 35.4 | 84 60.08 | | | AAA |
| | ATCM | 2571 | | | | 35.2 | 15 58.94 | 2 61.109 | 1.00 51.23 | |
| | ATOM | 2572 | O | 1 ASN | 323 | | EE 60 00 | | | AAA |
| | ATOM | | NT | 2 ASN | 323 | 36.4 | 55 60.80 | • | | AAA |
| | AIUM | | | | | 33.0 | 27 61.17 | 60.82 | 4 1.00 34.03 | |
| | | | | | | - - · | | | | |

| ATOM 2575 0 ASN 324 33.51 62.21 760.395 0.075 1.00 34.06 AAAA ATOM 2576 R ASN 324 33.551 62.270 58.995 1.00 31.06 AAAA ATOM 2578 C ASN 324 33.385 62.720 58.995 1.00 31.06 AAAA ATOM 2578 C ASN 324 33.385 62.720 58.995 1.00 31.06 AAAA ATOM 2578 C ASN 324 33.285 62.720 58.995 1.00 31.06 AAAA ATOM 2578 C ASN 324 32.974 65.163 59.450 1.00 35.07 AAAA ATOM 2580 OI ASN 324 33.555 66.008 60.291 1.00 39.55 AAAA ATOM 2580 ND ASN 324 33.555 66.008 60.291 1.00 39.12 AAAA ATOM 2581 ND2 ASN 324 33.555 66.008 60.291 1.00 39.12 AAAA ATOM 2582 C ASN 324 33.451 61.483 56.941 1.00 31.91 AAAA ATOM 2583 ND2 ASN 324 33.451 61.483 56.941 1.00 31.91 AAAA ATOM 2585 C ASN 324 33.451 61.483 56.941 1.00 31.91 AAAA ATOM 2585 C ASN 324 33.451 61.483 56.941 1.00 31.91 AAAA ATOM 2585 C LYS 325 35.991 60.538 57.333 1.00 29.55 AAAAA ATOM 2586 C LYS 325 38.250 59.386 59.7004 1.00 44.83 AAAA ATOM 2586 C LYS 325 38.250 59.386 57.004 1.00 44.83 AAAA ATOM 2589 C LYS 325 38.250 59.386 59.7004 1.00 44.83 AAAA ATOM 2589 C LYS 325 35.615 59.991 60.873 57.561 1.00 54.02 AAAA ATOM 2589 C LYS 325 35.616 58.85 59.998 00.00 37.43 AAAA ATOM 2589 C LYS 325 35.616 59.279 57.008 1.00 54.02 AAAA ATOM 2589 C LYS 325 35.616 59.279 57.008 1.00 54.02 AAAA ATOM 2593 C ALA AAA 3AA ATOM 2595 C AAAA 3AA ATOM 2596 C AAAA 326 33.600 58.700 39.700 30.00 31.00 30.30 AAAA ATOM 2597 C AAAA 326 33.600 58.700 39.700 30.3 | | | | | | • | | | | AAAA |
|--|-------|------|----|--------|-----|--------|-----------|-----------|------------|------|
| APPEN 2576 N ASN 324 33.551 62.317 08.985 1.00 31.06 AAAA AAAA AAAOM 2577 CA ASN 324 33.868 64.155 58.764 1.00 31.06 AAAA AAAA AAOM 2578 CB ASN 324 33.868 64.155 58.764 1.00 35.75 AAAA AAAA AAAA ACOM 2579 CG ASN 324 31.765 65.189 59.266 1.00 35.55 AAAAA ACOM 2580 OX ASN 324 31.555 66.008 60.261 1.00 39.15 AAAAA ACOM 2580 OX ASN 324 31.555 66.008 60.261 1.00 39.12 AAAAA ACOM 2580 OX ASN 324 31.555 66.008 60.261 1.00 39.12 AAAAA ACOM 2580 OX ASN 324 31.555 66.008 60.261 1.00 39.12 AAAAA ACOM 2580 OX ASN 324 31.555 66.008 60.261 1.00 39.12 AAAAA ACOM 2585 OX LYS 325 33.595 66.008 60.261 1.00 39.12 AAAAA ACOM 2586 CA LYS 325 33.595 66.008 60.261 1.00 31.91 AAAAA ACOM 2586 CA LYS 325 33.595 66.008 67.704 1.00 21.773 AAAAA ACOM 2586 CB LYS 325 33.595 66.008 57.004 1.00 41.84 AAAAA ACOM 2586 CB LYS 325 33.694 69.305 57.004 1.00 41.84 AAAAA ACOM 2589 CE LYS 325 33.694 69.305 57.004 1.00 41.84 AAAAA ACOM 2589 CE LYS 325 33.694 69.305 57.561 1.00 50.89 AAAAA ACOM 2590 CX LYS 325 33.606 58.72 58.142 1.00 27.99 AAAAA ACOM 2590 CX LYS 325 33.606 58.72 58.142 1.00 27.99 AAAAA ACOM 2592 CX LYS 325 33.4602 59.279 57.078 1.00 27.99 AAAAA ACOM 2595 CX LYS 325 33.4602 59.279 57.078 1.00 27.97 AAAAA ACOM 2595 CX LYS 325 33.4602 59.279 57.078 1.00 27.97 AAAAA ACOM 2595 CX LYS 327 30.502 59.279 57.078 1.00 27.77 AAAAA ACOM 2595 CX LYS 327 30.502 59.279 57.078 1.00 27.77 AAAAA ACOM 2595 CX LYS 327 30.502 59.279 59.428 1.00 31.80 AAAAA ACOM 2595 CX LYS 327 30.502 59.279 59.428 1.00 31.80 | 3 mov | 2575 | 0 | ASN | 323 | 32.429 | | | | |
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| ATOM 2588 CD LYS 325 39.684 9.435 57.561 1.00 54.82 AAAA ATOM 2599 NZ LYS 325 40.191 60.873 57.561 1.00 54.82 AAAA ATOM 2591 CL LYS 325 35.161 59.279 57.078 1.00 27.99 AAAA ATOM 2592 C LYS 325 35.161 59.279 57.078 1.00 27.99 AAAA ATOM 2592 C LYS 325 35.161 59.279 57.078 1.00 27.99 AAAA ATOM 2592 C LYS 325 35.161 59.279 57.078 1.00 27.99 AAAA ATOM 2593 C AAAA 326 33.781 57.506 58.030 1.00 24.38 AAAA ATOM 2595 CB ALA 326 33.781 57.506 58.030 1.00 24.38 AAAA ATOM 2595 C AAAA 326 33.781 57.506 58.030 1.00 24.38 AAAA ATOM 2595 C AAAA 326 32.478 57.709 57.231 1.00 25.78 AAAA ATOM 2595 C AAAA 326 32.478 57.709 57.231 1.00 25.78 AAAA ATOM 2595 C AAAA 326 32.478 57.09 57.09 57.231 1.00 25.78 AAAA ATOM 2595 C AAAA 326 32.478 57.09 57.231 1.00 25.78 AAAA ATOM 2595 C ALYS 327 30.502 59.027 56.758 1.00 27.31 AAAA ATOM 2590 CA LYS 327 30.502 59.027 56.758 1.00 27.31 AAAA ATOM 2590 CA LYS 327 29.759 60.251 57.333 1.00 28.67 AAAA ATOM 2500 CE LYS 327 29.759 60.251 57.333 1.00 28.67 AAAA ATOM 2600 CE LYS 327 29.991 60.209 58.812 1.00 36.72 AAAA ATOM 2600 CE LYS 327 28.643 61.807 59.255 1.00 40.34 AAAA ATOM 2600 CE LYS 327 30.092 59.244 55.269 1.00 27.76 AAAA ATOM 2600 CE LYS 327 30.092 59.244 55.269 1.00 27.76 AAAA ATOM 2600 CE LYS 327 30.092 59.244 55.269 1.00 27.76 AAAA ATOM 2600 CE LYS 327 30.092 59.244 55.269 1.00 27.76 AAAA ATOM 2600 CE LYS 327 30.092 59.244 55.269 1.00 27.76 AAAA ATOM 2600 CE LYS 327 30.992 59.244 55.269 1.00 27.76 AAAA ATOM 2601 CC GLU 328 33.294 64.00 25.555 51.561 1.00 47.67 AAAA ATOM 2601 CC GLU 328 33.294 64.00 25.555 51.561 1.00 27.76 AAAA ATOM 2601 CC GLU 328 33.295 64.007 55.550 71.00 47.50 AAAA ATOM 2601 CC GLU 328 33.295 64.007 52.951 1.00 30.23 30 AAAA ATOM 2601 CC GLU 328 33.295 64.007 52.951 1.00 32.30 AAAA ATOM 2601 CC GLU 328 33.295 64.007 52.951 1.00 32.30 AAAA ATOM 2601 CC GLU 328 33.295 64.007 52.951 1.00 32.30 AAAA ATOM 2602 CD LEU 328 33.796 60.055 51.561 1.00 27.76 AAAA ATOM 2602 CD LEU 328 33.796 60.055 51.561 1.00 22.570 AAAA ATOM 2602 CD LEU 328 33.796 50.055 51.651 1.00 32.30 AAAA | | | | | | | | | | |
| ATOM 2599 NZ LYS 325 40.91 60.980 57.969 1.00 65.70 AAAA ATOM 2591 C LYS 325 35.161 98.7936 57.969 1.00 65.70 AAAA ATOM 2592 NA LA 326 34.602 88.721 58.142 1.00 26.07 AAAA ATOM 2593 N ALA 326 34.602 88.721 58.142 1.00 26.07 AAAA ATOM 2595 CB ALA 326 33.470 56.982 59.428 1.00 27.34 AAAA ATOM 2595 CB ALA 326 33.470 56.982 59.428 1.00 27.34 AAAA ATOM 2596 C ALA 326 32.478 75.700 57.231 1.00 25.78 AAAA ATOM 2597 C ALA 326 32.478 75.700 57.231 1.00 25.78 AAAA ATOM 2598 N LYS 327 31.749 38.790 57.496 1.00 27.37 AAAAA ATOM 2599 CA LA 326 32.131 56.890 57.496 1.00 27.31 AAAA ATOM 2599 CA 25.70 AAAA ATOM 2598 N LYS 327 30.502 99.027 56.758 1.00 28.56 AAAA ATOM 2599 CA LYS 327 30.502 99.027 56.758 1.00 28.56 AAAA ATOM 2590 CB LYS 327 29.491 60.209 58.812 1.00 36.72 AAAA ATOM 2500 CB LYS 327 29.491 60.209 58.812 1.00 36.72 AAAA ATOM 2601 CG LYS 327 29.491 60.209 58.812 1.00 36.72 AAAA ATOM 2601 CC LYS 327 28.643 61.407 59.255 1.00 40.34 AAAA ATOM 2601 CC LYS 327 28.645 61.594 60.769 1.00 37.91 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 27.75 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 27.75 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 27.75 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 27.75 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 27.75 AAAA ATOM 2606 C LYS 327 30.997 89.794 65.269 1.00 29.15 AAAA ATOM 2607 N GLU 328 31.829 60.015 54.972 1.00 31.59 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 40.27.76 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 32.776 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 32.776 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 32.776 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 32.776 AAAA ATOM 2607 N GLU 328 33.257 61.332 53.515 1.00 32.776 AAAA ATOM 2607 N GLU 328 33.764 60.775 54.032 1.00 27.75 AAAA ATOM 2607 N GLU 328 33.798 60.015 54.972 1.00 31.59 AAAA ATOM 2607 N GLU 328 33.798 60.015 54.972 1.00 31.59 AAAA ATOM 2607 N GLU 328 33.798 60.005 55.4972 1.00 31.59 AAAA ATOM 2618 O GLU 328 33.798 60.005 55.991 1.00 27.75 AAAA ATOM 261 | | | | | 325 | | | | 1.00 50.09 | |
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| ATOM 2591 O LYS 325 35.016 38.836 35.938 1.00 26.07 AAAA ATOM 2593 N ALA 126 34.602 58.721 58.142 1.00 26.07 AAAA ATOM 2594 CA ALA 326 33.781 57.506 58.030 1.00 24.38 AAAA ATOM 2595 CB ALA 326 33.781 57.506 58.030 1.00 27.34 AAAA ATOM 2595 C ALA 326 32.478 57.709 57.231 1.00 25.78 AAAA ATOM 2597 O ALA 326 32.478 57.709 57.231 1.00 25.78 AAAA ATOM 2598 N LYS 327 31.749 58.790 57.496 1.00 27.37 AAAA ATOM 2599 CA LYS 327 30.502 59.027 56.758 1.00 28.56 AAAA ATOM 2599 CA LYS 327 30.502 59.027 56.758 1.00 28.56 AAAA ATOM 2590 CB LYS 327 29.491 60.293 58.812 1.00 36.72 AAAA ATOM 2600 CB LYS 327 28.643 61.594 60.769 1.00 38.91 AAAA ATOM 2601 CC LYS 327 28.643 61.594 60.769 1.00 38.91 AAAA ATOM 2602 CD LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2605 C LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2606 CD LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2606 CD LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2607 N GUU 328 31.829 60.015 54.972 1.00 31.59 AAAA ATOM 2608 CB GUU 328 31.829 60.015 54.972 1.00 31.59 AAAA ATOM 2610 CB GUU 328 31.829 60.015 54.972 1.00 31.59 AAAA ATOM 2610 CB GUU 328 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2610 CB GUU 328 33.764 63.772 54.032 1.00 44.667 AAAA ATOM 2611 CD GUU 328 33.764 63.772 54.032 1.00 44.667 AAAA ATOM 2610 CB GUU 328 33.764 63.772 54.032 1.00 44.667 AAAA ATOM 2611 CD GUU 328 33.764 63.772 54.032 1.00 44.67.50 AAAA ATOM 2612 CD LEU 329 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2613 CD LEU 329 33.765 66.035 55.875 1.00 30.46 AAAA ATOM 2614 C GUU 328 33.765 66.035 55.868 1.00 27.76 AAAA ATOM 2615 C G LEU 329 33.765 66.035 55.868 1.00 27.76 AAAA ATOM 2610 C G GUU 328 33.765 66.035 57.91 1.00 30.46 AAAA ATOM 2610 C G GUU 328 33.765 66.505 53.588 1.00 22.30 AAAA ATOM 2610 C G GUU 328 33.765 66.505 53.588 1.00 22.30 AAAA ATOM 2610 C G GUU 328 33.765 66.035 57.91 1.00 30.46 AAAA ATOM 2610 C G GUU 328 33.765 66.035 57.91 1.00 30.46 AAAA ATOM 2610 C G LEU 329 33.765 66.000 57.91 1.00 30.46 AAAA ATOM 2620 C D LEU 329 32.74 55.86 55.86 55.86 50.87 1.00 27.76 AAAA ATOM | | | | | 325 | | 59.279 | | 1.00 27.95 | |
| ATOM 2594 CA ALA 326 ATOM 2594 CA ALA 326 ATOM 2595 CB ALA 326 ATOM 2595 CB ALA 326 ATOM 2595 CB ALA 326 ATOM 2597 O ALA 326 ATOM 2597 O ALA 326 ATOM 2598 N LYS 327 ATOM 2599 CA LYS 327 ATOM 2590 CB LYS 327 ATOM 2601 CG LYS 327 ATOM 2602 CD LYS 327 ATOM 2602 CD LYS 327 ATOM 2603 CE LYS 327 ATOM 2604 NZ LYS 327 ATOM 2605 C LYS 327 ATOM 2605 C LYS 327 ATOM 2606 C LYS 327 ATOM 2606 C LYS 327 ATOM 2607 N GLU 328 ATOM 2607 N GLU 328 ATOM 2608 CA GLU 328 ATOM 2608 CA GLU 328 ATOM 2609 CB GLU 328 ATOM 2610 CG GLU 328 ATOM 2611 CD GLU 328 ATOM 2612 CDI GLU 328 ATOM 2612 CDI GLU 328 ATOM 2613 CDZ GLU 328 ATOM 2614 C GLU 328 ATOM 2615 CDI GLU 328 ATOM 2616 CDI GLU 328 ATOM 2617 CA LEU 329 ATOM 2618 CB LEU 329 ATOM 2619 CG LEU 329 ATOM 2620 CDI LEU 330 ATOM 2621 CDI LEU 330 ATOM 2621 CDI LEU 330 ATOM 2621 CDI LEU 330 ATOM 2622 CL EU 330 ATOM 2623 C LEU 330 ATOM 2623 C LEU 330 ATOM 2624 N LEU 330 ATOM 2635 CG LEU 330 ATOM 2636 C RE SEL 330 ATOM 2637 CE LEU 330 ATOM 2638 C RE SEL 330 ATOM | | | | LYS · | 325 | | | | 1 00 26 07 | |
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| ATOM 2595 CB ALA 326 33.478 57.709 57.231 1.00 25.78 AAAA ATOM 2596 C ALA 326 32.131 56.890 56.369 1.00 27.37 AAAA ATOM 2597 O ALA 326 32.131 56.890 56.369 1.00 27.37 AAAA ATOM 2599 CA LYS 327 30.502 59.027 56.758 1.00 28.56 AAAA ATOM 2599 CA LYS 327 29.759 60.251 57.313 1.00 28.87 AAAA ATOM 2590 CE LYS 327 29.759 60.251 57.313 1.00 28.87 AAAA ATOM 2601 CE LYS 327 29.491 60.209 58.812 1.00 36.72 AAAA ATOM 2602 CD LYS 327 28.643 61.407 59.255 1.00 40.34 AAAA ATOM 2603 CE LYS 327 28.643 61.407 59.255 1.00 40.34 AAAA ATOM 2603 CE LYS 327 28.643 61.407 59.255 1.00 47.67 AAAA ATOM 2603 CE LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2605 C LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 O LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 O LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2608 CA GLU 328 32.167 60.265 53.581 1.00 28.93 AAAA ATOM 2608 CA GLU 328 32.167 60.265 53.581 1.00 28.93 AAAA ATOM 2608 CA GLU 328 32.167 60.265 53.581 1.00 28.93 AAAA ATOM 2609 CB GLU 328 33.276 61.332 53.515 1.00 47.50 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2610 CG GLU 328 32.256 58.753 51.704 1.00 47.50 AAAA ATOM 2613 022 GLU 328 32.256 58.753 51.704 1.00 42.24 AAAA ATOM 2613 022 GLU 328 32.256 58.753 51.704 1.00 24.99 AAAA ATOM 2613 022 GLU 328 32.256 58.753 51.704 1.00 24.99 AAAA ATOM 2616 C LEU 329 33.701 56.828 53.017 1.00 24.80 AAAA ATOM 2617 CA LEU 329 33.701 56.828 53.017 1.00 24.80 AAAA ATOM 2619 CG LEU 329 34.478 56.003 54.053 1.00 25.70 AAAA ATOM 2619 CG LEU 329 34.478 56.003 54.053 1.00 25.70 AAAA ATOM 2619 CG LEU 329 32.256 58.753 51.704 1.00 24.99 AAAA ATOM 2619 CG LEU 329 32.300 30.939 55.569 52.603 1.00 23.50 AAAA ATOM 2619 CG LEU 330 30.939 55.569 52.603 1.00 23.50 AAAA ATOM 2620 CD1 LEU 329 34.478 56.005 55.168 1.00 24.73 AAAA ATOM 2621 CD2 LEU 330 30.039 54.252 55.168 1.00 22.71 AAAA ATOM 2621 CD2 LEU 330 30.039 54.252 55.168 1.00 22.71 AAAA ATOM 2622 C LEU 330 30.939 55.569 52.600 1.00 23.55 AAAA ATOM 2623 | | | CA | ALA | 326 | | | | 1 00 27 34 | |
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| ATOM 2598 N LYS 327 30.502 59.027 56.758 1.00 27.31 AAAA ATOM 2599 CA LYS 327 30.502 59.027 56.758 1.00 28.56 AAAA ATOM 2599 CA LYS 327 29.491 60.209 58.812 1.00 36.72 AAAA ATOM 2600 CB LYS 327 28.643 61.407 59.255 1.00 40.34 AAAA ATOM 2602 CD LYS 327 28.645 61.594 60.769 1.00 38.91 AAAA ATOM 2603 CE LYS 327 28.645 61.594 60.769 1.00 38.91 AAAA ATOM 2604 NZ LYS 327 28.645 61.594 60.769 1.00 38.91 AAAA ATOM 2605 C LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 C LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 C LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 C LYS 327 30.097 58.719 54.393 1.00 27.76 AAAA ATOM 2606 C LYS 328 31.29 60.015 54.972 1.00 31.59 AAAA ATOM 2608 CA GLU 328 31.29 60.015 54.972 1.00 31.59 AAAA ATOM 2608 CA GLU 328 33.257 61.332 53.515 1.00 32.30 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 47.50 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 47.50 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 47.50 AAAA ATOM 2610 CG GLU 328 33.984 64.402 55.087 1.00 42.24 AAAA ATOM 2613 OE2 GLU 328 33.257 64.037 52.951 1.00 56.88 AAAA ATOM 2613 OE2 GLU 328 33.264 64.402 55.087 1.00 42.24 AAAA ATOM 2613 OE2 GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2613 OE2 GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2615 O GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2616 CG GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2617 CA LEU 329 33.701 56.828 53.017 1.00 24.93 AAAA ATOM 2617 CA LEU 329 33.701 56.828 53.017 1.00 24.93 AAAA ATOM 2619 CG LEU 329 34.478 56.059 52.603 1.00 22.57 AAAA ATOM 2619 CG LEU 329 34.478 56.059 52.603 1.00 22.57 AAAA ATOM 2620 CDI LEU 329 34.478 56.059 52.603 1.00 23.50 AAAA ATOM 2621 CD LEU 330 30.289 55.168 1.00 24.73 AAAA ATOM 2620 CDI LEU 330 30.289 55.145 53.240 1.00 25.66 AAAA ATOM 2620 CDI LEU 330 30.39 54.252 51.10 0.0 26.65 AAAA ATOM 2621 CD LEU 330 30.39 54.252 51.600 1.00 23.50 AAAA ATOM 2622 CD LEU 330 30.93 54.252 55.660 51.252 1.00 26.65 AAAA ATOM 2623 CD LEU 330 30.93 59.556 55.168 1.00 22.77 AAAA ATOM 2623 CD LEU 330 30. | | | С | ALA | 326 | | | | 1.00 23.70 | |
| ATOM 2598 N LYS 327 31.749 58.795 56.758 1.00 28.56 AAAA AAAA ATOM 2599 CA LYS 327 29.759 60.251 57.313 1.00 28.67 AAAAA ATOM 2600 CB LYS 327 29.491 60.209 58.812 1.00 36.72 AAAAA ATOM 2601 CG LYS 327 28.643 61.407 59.255 1.00 40.34 AAAAA ATOM 2604 NZ LYS 327 28.645 61.594 60.769 1.00 38.91 AAAAA ATOM 2604 NZ LYS 327 28.645 61.594 60.769 1.00 38.91 AAAAA ATOM 2605 C LYS 327 30.792 59.244 55.269 1.00 27.76 AAAAA ATOM 2605 C LYS 327 30.992 59.244 55.269 1.00 27.76 AAAAA ATOM 2606 O LYS 327 30.992 59.244 55.269 1.00 27.76 AAAAA ATOM 2607 N GLU 328 31.829 60.015 54.972 1.00 31.59 AAAAA ATOM 2608 CB GLU 328 33.257 61.332 53.515 1.00 28.93 AAAA ATOM 2609 CB GLU 328 33.257 61.332 53.515 1.00 28.93 AAAA ATOM 2610 CG GLU 328 33.267 61.332 53.515 1.00 32.30 AAAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 46.67 AAAAA ATOM 2611 CD GLU 328 33.764 63.772 54.032 1.00 42.24 AAAAA ATOM 2613 OE2 GLU 328 33.984 64.402 55.087 1.00 42.24 AAAAA ATOM 2613 OE2 GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2614 C GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2615 O GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2616 N LEU 329 33.792 58.112 53.584 1.00 24.93 AAAA ATOM 2617 CA LEU 329 33.791 56.828 53.017 1.00 24.93 AAAA ATOM 2618 CB LEU 329 33.791 56.828 53.017 1.00 24.93 AAAA ATOM 2617 CA LEU 329 33.792 58.112 53.584 1.00 24.93 AAAA ATOM 2618 CB LEU 329 34.730 54.522 53.703 1.00 19.71 AAAAA ATOM 2620 CDL LEU 329 35.569 54.413 52.430 1.00 25.70 AAAAA ATOM 2621 CD LEU 329 32.715 56.095 51.453 1.00 25.70 AAAAA ATOM 2622 C LEU 329 34.730 56.095 51.452 1.00 25.26 AAAAA ATOM 2622 C LEU 329 34.730 56.095 51.452 1.00 25.26 AAAAA ATOM 2622 C LEU 330 30.289 55.145 53.249 1.00 23.95 AAAAA ATOM 2623 C LEU 330 30.399 54.252 55.145 50.00 25.25 AAAAA ATOM 2628 CDL LEU 330 30.399 54.252 55.145 50.00 25.25 AAAAA ATOM 2629 CD2 LEU 330 30.399 54.252 55.145 50.00 25.25 AAAAA ATOM 2629 CD2 LEU 330 30.399 54.252 55.145 50.00 25.25 AAAAA ATOM 2629 CD2 LEU 330 30.599 55.145 50.00 51.252 1.00 26.65 AAAAA ATOM 2636 C LYS 331 29.404 57.7097 52.11 | | | 0 | ALA | 326 | | | | 1 00 27 31 | |
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| ATOM 2601 CG LYS 327 29.69 60.205 58.812 1.00 36.72 AAAA ATOM 2602 CD LYS 327 28.643 61.407 59.255 1.00 40.34 AAAA ATOM 2602 CD LYS 327 28.643 61.594 60.769 1.00 38.91 AAAA ATOM 2602 CD LYS 327 28.645 61.594 60.6769 1.00 38.91 AAAA ATOM 2602 CD LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2606 CD LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2606 CD LYS 327 30.997 58.719 54.393 1.00 27.76 AAAA ATOM 2607 N GLU 328 32.167 60.265 53.581 1.00 28.91 AAAA ATOM 2608 CA GLU 328 32.167 60.265 53.581 1.00 28.91 AAAA ATOM 2609 CB GLU 328 32.745 62.652 54.067 1.00 32.30 AAAA ATOM 2609 CB GLU 328 32.745 62.652 54.067 1.00 46.67 AAAA ATOM 2610 CG GLU 328 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2611 CD GLU 328 33.984 64.402 55.087 1.00 46.67 AAAA ATOM 2612 OE1 GLU 328 33.984 64.402 55.087 1.00 46.67 AAAA ATOM 2613 OE2 GLU 328 33.984 64.402 55.087 1.00 30.46 AAAA ATOM 2614 C GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2615 O GLU 328 32.226 58.753 51.704 1.00 24.93 AAAA ATOM 2617 CA LEU 329 33.701 56.828 53.017 1.00 24.93 AAAA ATOM 2618 CB LEU 329 34.478 56.003 54.053 1.00 25.70 AAAA ATOM 2619 CG LEU 329 34.478 56.003 54.053 1.00 25.50 AAAA ATOM 2620 CD1 LEU 329 34.478 56.003 54.053 1.00 25.50 AAAA ATOM 2621 CD2 LEU 329 34.730 54.452 53.703 1.00 19.71 AAAA ATOM 2621 CD2 LEU 329 32.413 55.684 1.00 24.93 AAAA ATOM 2620 CD1 LEU 329 32.413 55.685 1.00 24.73 AAAA ATOM 2620 CD1 LEU 329 32.413 56.059 52.603 1.00 23.50 AAAA ATOM 2620 CD1 LEU 329 32.310 55.650 51.453 1.00 25.50 AAAA ATOM 2620 CD1 LEU 329 32.310 55.650 51.453 1.00 25.50 AAAA ATOM 2620 CD1 LEU 330 30.289 55.145 53.359 1.00 23.50 AAAA ATOM 2623 C LEU 330 30.289 55.145 53.359 1.00 23.50 AAAA ATOM 2623 C LEU 330 30.399 55.145 53.599 1.00 23.50 AAAA ATOM 2623 C LEU 330 30.399 55.145 53.599 1.00 23.50 AAAA ATOM 2623 C LEU 330 30.399 55.145 53.599 1.00 23.50 AAAA ATOM 2628 CD1 LEU 330 30.399 55.145 53.599 1.00 23.50 AAAA ATOM 2628 CD1 LEU 330 30.399 55.145 53.599 1.00 23.50 AAAA ATOM 2628 CD1 LEU 330 30.399 55.145 50.2990 1.00 27.75 AAAA ATOM 2631 C LEU 330 30. | | | ÇA | LYS | | | | | 1 00 28 87 | AAAA |
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| ATOM 2604 NZ LYS 327 30.792 59.244 55.269 1.00 47.67 AAAA ATOM 2606 C LYS 327 30.792 59.244 55.269 1.00 29.15 AAAA ATOM 2606 C LYS 327 30.792 59.244 55.269 1.00 27.76 AAAA ATOM 2606 C LYS 327 30.997 58.719 54.393 1.00 27.76 AAAA ATOM 2607 N GLU 328 31.829 60.015 54.972 1.00 31.59 AAAA ATOM 2608 CA GLU 328 32.167 60.265 53.581 1.00 28.93 AAAA ATOM 2609 CB GLU 328 33.257 61.332 53.515 1.00 32.30 AAAA ATOM 2610 CG GLU 328 33.2745 62.652 54.067 1.00 47.50 AAAA ATOM 2611 CD GLU 328 33.764 63.772 54.032 1.00 46.67 AAAA ATOM 2613 022 GLU 328 33.984 64.402 55.087 1.00 42.24 AAAA ATOM 2613 022 GLU 328 33.984 64.402 55.087 1.00 42.24 AAAA ATOM 2613 022 GLU 328 33.257 58.975 52.871 1.00 30.46 AAAA ATOM 2616 N LEU 329 33.292 58.112 53.584 1.00 24.93 AAAA ATOM 2616 N LEU 329 33.701 56.828 53.017 1.00 44.93 AAAA ATOM 2617 CA LEU 329 33.701 56.828 53.017 1.00 24.93 AAAA ATOM 2618 CB LEU 329 34.478 56.003 54.053 1.00 25.70 AAAA ATOM 2619 CG LEU 329 .5.569 54.413 52.430 1.00 25.26 AAAA ATOM 2620 CD1 LEU 329 .5.569 54.413 52.430 1.00 25.26 AAAA ATOM 2622 C LEU 329 .5.569 54.413 52.430 1.00 25.26 AAAA ATOM 2622 C LEU 329 .5.569 54.413 52.430 1.00 25.26 AAAA ATOM 2622 C LEU 329 .5.569 54.413 52.430 1.00 25.26 AAAA ATOM 2622 C LEU 329 .5.569 55.441 55.309 1.00 23.02 AAAA ATOM 2622 C LEU 329 .5.569 55.441 55.309 1.00 23.02 AAAA ATOM 2622 C LEU 330 30.289 55.442 53.833 54.863 1.00 25.26 AAAA ATOM 2622 C LEU 330 30.289 55.442 53.833 54.863 1.00 25.26 AAAA ATOM 2622 C LEU 330 30.289 55.445 53.591 1.00 23.02 AAAA ATOM 2622 C LEU 330 30.039 54.252 55.642 1.00 23.02 AAAA ATOM 2623 C LEU 330 30.039 54.252 55.642 1.00 25.29 AAAA ATOM 2630 C LEU 330 30.039 54.252 55.168 1.00 29.529 AAAA ATOM 2630 C LEU 330 30.039 54.252 55.642 1.00 25.29 53 AAAA ATOM 2630 C LEU 330 30.588 52.905 55.168 1.00 29.53 AAAA ATOM 2637 CE LEU 330 30.588 6667 57.795 51.066 1.00 29.53 AAAA ATOM 2630 C LEU 330 28.968 55.060 51.252 1.00 26.65 AAAA ATOM 2631 C LEU 330 28.968 55.060 51.252 1.00 26.65 AAAA ATOM 2637 CE LYS 331 28.667 57.795 51.066 1.00 29.53 AAAA ATOM 2630 | | 2602 | CD | | | | | | 1.00 38.91 | AAAA |
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| ATOM 2625 CA LEU 330 | | | | | 330 | | | | 1.00 23.02 | |
| ATOM 2626 CB LEU 330 | | | | | | | | | | |
| ATOM 2627 CG LEU 330 | | | | | 330 | | | | | |
| ATOM 2628 CD1 LEU 330 28.984 54.053 55.168 1.00 22.44 AAAA ATOM 2629 CD2 LEU 330 29.491 55.769 52.113 1.00 26.94 AAAA ATOM 2631 0 LEU 330 28.968 55.060 51.252 1.00 26.65 AAAA ATOM 2631 N LYS 331 29.404 57.097 52.111 1.00 30.82 AAAA ATOM 2633 CA LYS 331 28.667 57.795 51.066 1.00 29.53 AAAA ATOM 2634 CB LYS 331 28.667 57.795 51.066 1.00 29.67 AAAA ATOM 2635 CG LYS 331 27.814 59.567 52.714 1.00 36.06 AAAA ATOM 2636 CD LYS 331 27.814 59.567 52.914 1.00 36.06 AAAA ATOM 2636 CD LYS 331 27.688 61.055 52.990 1.00 42.75 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.C7 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.C7 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 36.20 | | | | | 330 | 30.03 | | | | |
| ATOM 2629 CD2 LEU 330 | | | | | 330 | | | 55 56.744 | | |
| ATOM 2630 C LEU 330 29.491 55.765 52.990 1.00 26.65 AAAA AAAA ATOM 2631 C LYS 331 27.688 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2638 NZ LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 36.20 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 36.20 | | | | | 330 | 30.53 | | | | AAAA |
| ATOM 2631 O LEU 330 ATOM 2632 N LYS 331 ATOM 2633 CA LYS 331 ATOM 2634 CB LYS 331 ATOM 2635 CG LYS 331 ATOM 2636 CD LYS 331 ATOM 2637 CE LYS 331 ATOM 2638 NZ LYS 331 ATOM 2638 NZ LYS 331 ATOM 2639 C LYS 331 | | | | | 330 | 29.49 | | | | |
| ATOM 2632 N LYS 331 29.404 57.097 52.111 1.00 29.53 AAAA ATOM 2633 CA LYS 331 28.667 57.795 51.066 1.00 29.53 AAAA ATOM 2634 CB LYS 331 28.537 59.292 51.407 1.00 29.67 AAAA ATOM 2635 CG LYS 331 27.814 59.567 52.714 1.00 36.06 AAAA ATOM 2636 CD LYS 331 27.688 61.055 52.990 1.00 42.75 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA | | | | | 330 | 28.96 | | | | |
| ATOM 2633 CA LYS 331 28.667 57.793 51.407 1.00 29.67 AAAA ATOM 2634 CB LYS 331 28.537 59.292 51.407 1.00 36.06 AAAA ATOM 2635 CG LYS 331 27.814 59.567 52.714 1.00 36.06 AAAA ATOM 2636 CD LYS 331 27.688 61.055 52.990 1.00 42.75 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA | | | | | | 29.40 | | | | |
| ATOM 2634 CB LYS 331 28.537 59.292 31.00 36.06 AAAA ATOM 2635 CG LYS 331 27.814 59.567 52.714 1.00 36.06 AAAA ATOM 2636 CD LYS 331 27.688 61.055 52.990 1.00 42.75 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 36.20 AAAA | | | | | | 28.6 | | | | |
| ATOM 2635 CG LYS 331 27.814 59.567 52.990 1.00 42.75 AAAA ATOM 2636 CD LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 67.57 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 28.634 57.759 48.672 1.00 36.20 AAAA | | · · | | | 331 | 28.5 | | 54 SI.WU | | AAAA |
| ATOM 2636 CD LYS 331 27.688 61.055 32.950 1.00 53.98 AAAA ATOM 2637 CE LYS 331 26.828 61.737 51.939 1.00 53.98 AAAA ATOM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 67.57 AAAA ATOM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 28.634 57.759 48.672 1.00 36.20 AAAA | | | | | | 27.8 | | | | |
| ATCM 2637 CE LYS 331 26.624 63.185 52.234 1.00 67.57 AAAA ATCM 2638 NZ LYS 331 26.634 63.185 52.234 1.00 30.07 AAAA ATCM 2639 C LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATCM 2639 C LYS 331 29.315 57.759 48.672 1.00 36.20 AAAA | | | | | | | | | | |
| ATOM 2638 NZ LYS 331 29.315 57.628 49.692 1.00 30.07 AAAA ATOM 2639 C LYS 331 29.315 57.759 48.672 1.00 36.20 AAAA | | | | | | 26.8 | | | | |
| ATOM 2639 C LYS 331 28.634 57.759 48.672 1.00 36.20 AAAA | | | | LYS | | 26.6 | | | | |
| | | | | LYS | | | | | | AAAA |
| | | | 0 | LYS | 331 | 28.5 | ا ۱۰۱ و و | 25 30:31 | | • |

| | | | | | 205 | 49.657 | 1.00 30.08 | AAAA |
|--------------|------|----------|-------|-------------|--------|----------|---------------|------------------|
| | 2641 | 1 SER | 332 | | 57.305 | | 1.00 30.00 | AAAA |
| MOTA | | | - 332 | 31.322 | 57.153 | 48.385 | 1.00 33.35 | |
| ATOM | 2642 | CA SER | | • • • • • • | 57.312 | 48.590 | 1.00 40.36 | aaaa |
| ATOM | 2643 | CB SER | 332 | | | | 1.00 34.04 | AAAA |
| | | OG SER | 332 | | 56.169 | | | |
| MOTA | | | | 31.061 | 55.821 | | 1.00 37.72 | AAAA |
| ATOM | 2645 | C SER | 332 | | | 46.507 | 1.00 30.78 | AAAA |
| | 2646 | SER | 332 | | 55.661 | | 1 00 30 61 | AAAA |
| MOTA | | · | 333 | 30.521 | 54.865 | | 1.00 30.61 | |
| ATOM | 2647 | N ILE | | | 53.547 | 47.899 | 1.00 37.59 | AAAA |
| ATOM | 2648 | CA ILE | 333 | | | | 1.00 33.59 | AAAA |
| | | | . 333 | 29.901 | 52.551 | | | |
| MOTA | | | | | 51.146 | 48.442 | 1.00 37.05 | AAAA |
| ATCM | 2650 | CG2_ ILE | 333 | | | 50.065 | 1.00 38.95 | AAAA |
| | | CG1 ILE | 333 | | 52.564 | 50.005 | | AAAA |
| MOTA | _ | COI ILE | 333 | 30.706 | 51.727 | 51.282 | 1.00 46.83 | |
| ATOM | 2652 | CD1 ILE | | • • • | 53.620 | 46.998 | 1.00 43.41 | aaaa |
| ATOM | 2653 | C ILE | 333 ` | | | | 1.00 46.24 | AAAA |
| | | | 333 | 27.889 | 53.876 | 47.479 | 1.00 40.24 | |
| MOTA | | | | 29.158 | 53.423 | 45.696 | 1.00 47.97 | AAAA |
| ATOM | 2655 | n asp | 334 | | | 44.847 | 1.00 53.47 | - AAAA |
| | | CA ASP | 334 | 27.976 | 53.447 | | | AAAA |
| MOTA | | | 334 | 28.333 | 53.535 | 43.358. | 1.00 61.52 | |
| ATOM | 2657 | CB ASP | | | 52.406 | 42.897 | 1.00 64.75 | AAAA |
| ATOM | 2658 | CG ASP | 334 | 29.223 | | | 1.00 66.93 | AAAA |
| | | OD1 ASP | 334 | 29.379 | 52.248 | 41.566 | 1.00 00.55 | AAAA |
| MOTA | | | | 29.779 | 51.691 | 43.758 | 1.00 65.93 | |
| ATOM | 2660 | OD2 ASP | 334 | | 52.144 | 45.161 | 1.00 51.83 | AAAA |
| ATOM | 2661 | C ASP | 334 | 27.248 | | | 1.00 46.80 | AAAA |
| | | | 334 | 27.626 | 51.067 | 44.699 | 1.00 40.00 | |
| MOTA | 2662 | O ASP | | 26.215 | 52.249 | 45.986 | 1.00 54.96 | AAAA |
| MOTA | 2663 | N PHE | 335 | 20.213 | | | 1.00 50.60 | AAAA |
| | 2664 | CA PHE | 335 | 25.455 | 51.080 | | 1.00 30.00 | AAAA |
| MOTA | | | 335 | 25.413 | 51.003 | 47.920 | 1.00 39.55 | |
| MOTA | 2665 | CB PHE | | | 50.054 | 48.440 | 1.00 37.98 | aaaa |
| MOTA | 2666 | CG PHE | 335 | 24.380 | | | 1.00 46.72 | AAAA |
| | | CD1 PHE | 335 | 24.389 | 48.715 | 48.054 | 1.00 40.72 | |
| MOTA | 2667 | | | 23.362 | 50.506 | 49.262 | 1.00 34.23 | AAAA |
| MOTA | 2668 | CD2 PHE | 335 | | | 48.478 | 1.00 49.80 | AAAA |
| | 2669 | CE1 PHE | 335 | 23.389 | 47.842 | | 1.00 48.51 | AAAA |
| ATOM | | | 335 | 22.361 | 49.644 | 49.689 | 1.00 40.5 | |
| ATOM | 2670 | CE2 PHE | | 22.373 | 48.309 | 49.296 | 1.00 40.44 | AAAA |
| MOTA | 2671 | CZ PHE | 335 | | | 45.839 | 1.00 54.52 | AAAA |
| | 2672 | C PHE | 335 | 24.033 | 51.000 | | 1.00 51.52 | AAAA |
| MOTA | | | | 23.603 | 49.939 | 45.379 | 1.00 59.24 | |
| ATOM | 2673 | O PHE | 335 | 23.003 | 52.108 | | 1.00 50.94 | AAAA |
| ATOM | 2674 | N GLU | 336 | 23.302 | | | 1.00 57.05 | AAAA |
| | | | 336 | 21.923 | 52.119 | 45.406 | 1.00 37.03 | AAAA |
| MOTA | 2675 | | | 21.853 | 51.751 | 43.924 | 1.00 60.27 | |
| ATOM | 2676 | CB GLU | 336 | | | | 1.00 68.55 | AAAA |
| | 2677 | CG GLU | 336 | 20.430 | 51.627 | | | AAAA |
| MOTA | | | | 20.352 | 51.126 | 42.001 | 1.00 80.03 | |
| MOTA | 2678 | CD GLU | | 20.060 | 50.013 | | 1.00 84.64 | AAAA |
| ATOM | 2679 | OE1 GLU | 336 | 20.860 | | | 1.00 80.68 | AAAA |
| | | OE2 GLU | | 19.777 | 51.841 | | 1.00 00.00 | AAAA |
| MÒTA | 2680 | | | 21.065 | 51.135 | 46.201 | 1.00 55.73 | |
| MOTA | 2681 | C GLU | | | 49.917 | | 1.00 51.33 | ለ አአአ |
| ATOM | 2682 | O GLU | 336 | 21.219 | | | 1.00 49.54 | AAAA |
| | | | | 20.151 | 51.679 | 46.992 | | AAAA |
| MOTA | 2683 | | | 19.267 | 50.880 | 47.821 | 1.00 48.19 | |
| ATOM | 2684 | CA GLU | | | | | 1.00 47.73 | AAAA |
| | 2685 | CB GLU | 337 | 18.510 | 51.822 | · | 1.00 55.69 | AAAA |
| MOTA | 2005 | | | 18.084 | 51.205 | 50.077 | | • |
| MOTA | 2686 | | | 19.269 | 50.720 | 50.904 | 1.00 50.17 | AAAA |
| MOTA | 2687 | CD GLU | | | | | 1.00 36.03 | AAAA |
| | 2688 | OE1 GLU | 337 | 20.111 | 51.548 | | 1.00 51.25 | AAAA |
| ATOM | | 200 011 | | 19.358 | 49.494 | 51.105 | 1.00 51.25 | |
| MOTA | 2689 | OE2 GLU | | 10 304 | 50.083 | | 1.00 49.13 | AAAA |
| ATOM | 2690 | C GLU | | 18.294 | | | | AAAA |
| | | O GLU | | 17.816 | 50.588 | | | AAAA |
| ATOM | 2691 | | | 18.015 | 48.837 | 7 47.313 | 1.00 48.15 | |
| MOTA | 2692 | N PHE | | | 48.000 | | | AAA A |
| | 2693 | CA PHE | 338 | 17.092 | | | | AAAA |
| MOTA | | | | 16.870 | 46.658 | | | |
| MOTA | 2694 | CB PHE | | | | | 1.00 57.22 | LAAA |
| ATOM | 2695 | CG PHI | 338 | 15.883 | | | | LAA A |
| | | CD1 PH | | 16.115 | 45.36 | | | AAA |
| Mota | 2696 | | | 14.699 | | 8 47.171 | | |
| MOTA | 2697 | CD2 PHI | ≘ 338 | | | | | LAAA |
| | | CE1 PH | E 338 | 15.185 | | | | LAA A |
| MOTA | | | | 13.758 | 44.62 | 4 46.497 | | AAAi |
| MOTA | 2699 | CE2 PH | | 14.002 | | | 1.00 57.18 | |
| ATOM | | CZ PH | | | | | | aaai |
| | | C PH | E 338 | 15.755 | 48.71 | | | AAA |
| ATOM | | | | 15.274 | | 0 45.263 | | |
| ATOM | | O PH | | | | | l 1.00 40.38 | AAA |
| | | N AS | p 339 | 15.154 | | | 0 07 | AAA |
| MOTA | | | | 13.890 | 49.82 | | | AAA |
| ATOM | 2704 | | | 13.270 | 49.82 | 1 48.886 | 1.00 53.23 | |
| ATOM | | CB AS | | 13.470 | | | 3 1.00 57.40 | AAA |
| ATOM ATOM | | CG AS | p 339 | 12.000 | 50.65 | | - | • |
| אוו דיני ב | | | | | | | | |

| 3 most | 2207 | 001 | ASP | 339 | 12.039 | 51.858 | 48.616 | 1.00 53.79 | AAAA |
|--------|------|-----|------|-------|---------|-----------------|----------|------------|-------------|
| MOTA | 2707 | | | | | | | _ | |
| MOTA | 2708 | OD2 | ASP | 339 | 10.963 | 50.118 | 49.401 | 1.00 51.15 | AAAA |
| | 2709 | С | ASP | 339 | 14.215 | 51.248 | 47.076 | 1.00 55.06 | AAAA |
| MOTA | | | | | | | | 1.00 56.47 | AAAA |
| MOTA | 2710 | 0 | ASP | 339 | 14.994 | 51.922 | 47.748 | | |
| ATOM | 2711 | N | ASP | 340 | 13.623 | 51.708 | 45.978 | 1.00 58.46 | AAAA |
| | | | | | | | 45.484 | 1.00 67.72 | AAAA |
| ATOM | 2712 | CA | ASP | 340 | 13.874 | 53.059 | | | |
| * mon | 2713 | CB | ASP | 340 | 12.683 | 53.559 | 44.664 | 1.00 71.52 | AAAA |
| MOTA | | | | | | | | 1.00 79.72 | AAAA |
| MOTA | 2714 | CG | ASP | 340 | 12.611 | 52.913 | 43.295 | | |
| | 2715 | OD1 | a CD | 340 | 12.528 | 51.667 | 43.224 | 1.00 86.74 | AAAA |
| MOTA | | | | | | | | 1.00 83.40 | AAAA |
| ATOM | 2716 | OD2 | ASP | 340 | 12.640 | 53.655 | 42.288 | | |
| | 2717 | С | ASP | 340 | 14.209 | 54.072 | 46.572 | 1.00 69.65 | AAAA |
| MOTA | | | | | | | 46.463 | 1.00 70.13 | AAAA |
| MOTA | 2718 | 0 | ASP | 340 | 15.204 | 54.794 | | • | |
| MOTA | 2719 | N | GLU | 341 | 13.392 | 54.130 | 47.620 | 1.00 67.11 | AAAA |
| | | | | | | 55.077 | 48.689 | 1.00 67.87 | AAAA |
| ATOM | 2720 | CA | GLU | 341 | | | | | |
| MOTA | 2721 | CB | GLU | 341 | 13.195 | 56.478 | 48.278 | 1.00 74.87 | AAAA |
| | | | | | 13.502 | 57.576 | 49.298 | 1.00 82.72 | AAAA |
| MOTA | 2722 | CG | GLU | 341 | | | | | |
| MOTA | 2723 | CD | GLU | 341 | 13.162 | 58.974 | 48.790 | 1.00 90.80 | AAAA |
| | | | GLU | 341 | 11.988 | 59.215 | 48.431 | 1.00 90.38 | AAAA |
| ATOM | 2724 | | | | | | | | |
| MOTA | 2725 | OE2 | GLU | 341 | 14.072 | 59.835 | 48.752 | 1.00 93.36 | AAAA |
| | 2726 | С | GLU | 341 | 13.101 | 54.719 | 50.058 | 1.00 60.22 | AAAA |
| MOTA | | | | | | | | 1.00 58.81 | AAAA |
| MOTA | 2727 | 0 | GLU | 341 | 11.929 | 54.955 | 50.347 | | |
| | 2728 | N | VAL | 342 | 13.956 | 54.144 | 50.897 | 1.00 57.28 | AAAA |
| ATOM | | | | | | | 52.262 | 1.00 52.09 | AAAA |
| ATOM | 2729 | CA | VAL | 342 | 13.594 | 53.781 | | | |
| | 2730 | CB | VAL | 342 | 14.195 | 52.419 | 52.669 | 1.00 53.17 | AAAA |
| MOTA | | | | | | | 54.070 | 1.00 46.16 | AAAA |
| MOTA | 2731 | CG1 | VAL | 342 | 13.730 | 52.042 | | | |
| ATOM | 2732 | CG2 | VAL | 342 | 13.815 | 51.356 | 51.663 | 1.00 59.09 | AAAA |
| | | | | | 14.263 | 54.843 | 53.124 | 1.00 53.31 | AAAA |
| ATOM | 2733 | С | VAL | 342 | | | | | |
| MOTA | 2734 | 0 | VAL | 342 | 13.763 | 55.230 | 54.185 | 1.00 57.79 | AAAA |
| | 2735 | | ASP | 343 | 15.398 | 55.306 | 52.610 | 1.00 46.24 | AAAA |
| MOTA | | N | | | | | | | AAAA |
| MOTA | 2736 | CA | ASP | 343 | 16.268 | 56.289 | 53.243 | 1.00 42.60 | - |
| | 2737 | CB | ASP | 343 | 15.521 | 57.510 | 53.781 | 1.00 43.88 | AAAA |
| ATOM | | | | | | | | 1.00 46.82 | AAAA |
| ATOM | 2738 | CG | ASP | 343 | 16.480 | 58.581 | 54.290 | | |
| MOTA | 2739 | OD1 | ASP | 343 | 16.028 | 59.581 | 54.887 | 1.00 46.16 | AAAA |
| | | | | | | 58.414 | 54.075 | 1.00 33.01 | AAAA |
| MOTA | 2740 | OD2 | ASP | 343 · | 17.700 | | | | |
| ATOM | 2741 | C | ASP | 343 | 17.012 | 55 <i>.</i> 636 | 54.395 | 1.00 35.45 | AAAA |
| | | | | | 16.487 | 55.480 | 55.502 | 1.00 29.39 | AAAA |
| MOTA | 2742 | 0 | ASP | 343 | | | | | |
| ATOM | 2743 | N | ARG | 344 | 18.247 | 55.249 | 54.124 | 1.00 30.51 | AAAA |
| | | | ARG | 344 | 19.059 | 54.613 | 55.140 | 1.00 29.43 | AAAA |
| MOTA | 2744 | CA | | | | | | | AAAA |
| ATOM | 2745 | CB | ARG | 344 | 19.736 | 53.377 | 54.561 | 1.00 30.10 | |
| | 2746 | CG | ARG | 344 | 18.803 | 52.258 | 54.180 | 1.00 33.95 | AAAA |
| MOTA | | | | | | 51.770 | 55.365 | 1.00 20.92 | AAAA |
| MOTA | 2747 | CD | ARG | 344 | 17.981 | | | | |
| MOTA | 2748 | NE | ARG | 344 | 17.120 | 50.673 | 54.936 | 1.00 29.72 | AAAA |
| | | | | 344 | 16.110 | 50.176 | 55.639 | 1.00 29.13 | AAAA |
| ATOM | 2749 | CZ | ARG | | | | | | AAAA |
| ATOM | 2750 | NHl | ARG | 344 | 15.805 | 50.668 | 56.835 | 1.00 29.63 | |
| | 2751 | | ARG | 344 | 15.379 | 49.198 | 55.120 | 1.00 27.19 | AAAA: |
| ATOM | | | | | | | | 1.00 34.31 | AAAA |
| ATOM | 2752 | C | ARG | 344 | 20.116 | 55.~69 | 55.660 | | |
| ATOM | 2753 | 0 | ARG | 344 | 21.005 | 5557 | 56.391 | 1.00 29.09 | AAAA |
| | | | | | 20.011 | 56. 45 | 55.294 | 1.00 28.34 | AAAA |
| ATOM | 2754 | N | SER | 345 | | | | | |
| MOTA | 2755 | CA | SER | 345 | 20.999 | 57.839 | 55.715. | 1.00 30.95 | AAAA |
| | | | | 345 | 20.669 | 59.199 | 55.109 | 1.00 29.56 | AAAA |
| MOTA | 2756 | CB | SER | | | | | | |
| ATOM | 2757 | OG | SER | 345 | 19.429 | 59.648 | 55.610 | 1.00 29.38 | AAAA |
| | | | SER | 345 . | 21.137 | 57.988 | 57.230 | 1.00 30.92 | AAA |
| ATOM | 2758 | .C | | | | | | | LAAA |
| ATOM | 2759 | 0 | SER | 345 | 22.155 | 58.488 | 57.718 | 1.00 31.15 | |
| | 2760 | N | TYR | 346 | 20.116 | 57.576 | 57.975 | 1.00 25.64 | LAAA |
| MOTA | | | | - | | | | 1.00 26.81 | LAAA |
| ATOM | 2761 | CA | TYR | 346 | 20.158 | 57.659 | 59.433 | | |
| ATOM | 2762 | CB | TYR | 346 | 18.823 | 57.189 | 60.006 | 1.00 34.41 | LAAA |
| - | | | | | | 55.723 | 59.716 | 1.00 27.35 | LAAA |
| ATOM | 2763 | CG | TYR | 346 | 18.529 | | | | |
| ATOM | 2764 | | TYR | 346 | 19.003 | 54.708 | 60.556 | 1.00 24.87 | AAAi |
| | | | | | 18.744 | 53.352 | 60.278 | 1.00 28.05 | AAA: |
| ATOM | 2765 | CEL | TYR | 346 | | | | | |
| ATOM | 2766 | CD2 | TYR | 346 | 17.795 | 55.358 | 58.588 | 1.00 27.70 | AAA |
| | | | | | 17.533 | 54.008 | - 58.297 | 1.00 26.59 | AAA. |
| ATOM | 2767 | CE2 | TYR | 346 | | | | | AAA |
| ATOM | 2768 | CZ | TYR | 346 | .18.008 | 53.015 | 59.145 | 1.00 33.75 | |
| | | | TYR | 346 | 17.737 | 51.691 | 58.855 | 1.00 26.06 | AAA |
| MOTA | 2769 | ОН | | | | | | 1.00 25.57 | AAA |
| ATCM | 2770 | С | TYR | 346 | 21.277 | 56.766 | 59.977 | 1.00 23.37 | |
| | 2771 | ō | TYR | 346 | 21.769 | 56.970 | 61.085 | 1.00 28.07 | AAA |
| ATOM | | | | | | 55.761 | 59.198 | 1.00 29.08 | AAA |
| ATCM | 2772 | N | MET | 347 | 21.666 | 22.101 | J3.130 | 1.00 25.00 | |
| | | | | | • | | - | | • |
| • | | | | | | | | | |

| 3 TOM | 2773 | CA | MET | 347 | 22.720 | 54.837 | 59.622 | 1.00 24.19 | AAAA |
|--------------|--------------|----------|------------|------------|--------|-------------|--------|------------|------|
| MOTA | 2774 | CB | MET | 347 | 22.844 | 53.678 | 58.628 | 1.00 24.87 | AAAA |
| MOTA MOTA | 2775 | CG | MET | 347 | 21.609 | 52.806 | 58.543 | 1.00 23.66 | AAAA |
| ATOM | 2776 | SD | MET | 347 | 21.780 | 51.503 | 57.267 | 1.00 27.02 | AAAA |
| ATOM | 2777 | CE. | MET | 347 | 22.115 | 52.375 | 55.896 | 1.00 37.69 | AAAA |
| | 2778 | C | MET | 347 | 24.054 | 55.540 | 59.737 | 1.00 29.45 | AAAA |
| MOTA | 2779 | 0 | MET | 347 | 24.937 | 55.092 | 60.479 | 1.00 28.08 | AAAA |
| ATOM | 2779 | N | LEU | 348 | 24.188 | 56.650 | 59.007 | 1.00 23.71 | AAAA |
| MOTA | | | LEU | 348 | 25.418 | 57.446 | 58.998 | 1.00 34.11 | AAAA |
| MOTA | 2781 | CA CB | LEU | 348 | 25.463 | 58.351 | 57.757 | 1.00 25.37 | AAAA |
| MOTA | 2782 | CG | LEU | 348 | 25.320 | 57.785 | 56.344 | 1.00 30.38 | AAAA |
| MOTA | 2783 | | LEU | 348 | 25.307 | 58.944 | 55.340 | 1.00 27.44 | AAAA |
| ATOM | 2784 | | LEU | 348 | 26.459 | 56.814 | 56.041 | 1.00 36.44 | AAAA |
| ATOM | 2785 | | LEU | 348 | 25.507 | 58.332 | 60.237 | 1.00 36.09 | AAAA |
| ATOM | 2786 | C | | 348 | 26.561 | 58.894 | 60.539 | 1.00 33.30 | AAAA |
| MOTA | 2787 | 0 | LEU | 349 | 24.394 | 58.445 | 60.953 | 1.00 30.51 | AAAA |
| MOTA | 2788 | N | GLU GLU | 349 | 24.313 | 59.292 | 62.136 | 1.00 35.53 | AAAA |
| ATOM | 2789 | CA | GLU | 349 | 22.908 | 59.896 | 62.217 | 1.00 31.35 | AAAA |
| ATOM | 2790 | CB | GLU | 349 | 22.518 | 60.717 | 61.006 | 1.00 29.09 | AAAA |
| MOTA | 2791 | CG CD | GLU | 349 | 23.481 | 61.859 | 60.746 | 1.00 31.78 | AAAA |
| MOTA | 2792 | | GLU | 349 | 23.937 | 62.476 | 61.730 | 1.00 30.98 | AAAA |
| MOTA | 2793 | | | 349 | 23.766 | 62.155 | 59.569 | 1.00 30.67 | AAAA |
| MOTA | 2794 | | GLU | 349 | 24.663 | 58.633 | 63.471 | 1.00 38.48 | AAAA |
| ATOM | 2795 | 0 | GLU | 349 | 24.727 | 59.303 | 64.502 | 1.00 40.12 | AAAA |
| MOTA | 2796 | .0 | GLU | 350 | 24.878 | 57.326 | 63.461 | 1.00 33.58 | AAAA |
| ATOM | 2797 | N | THR | 350 | 25.221 | 56.612 | 64.681 | 1.00 29.74 | AAAA |
| MOTA | 2798 | CA | THR | 350 | 23.992 | 56.363 | 65.559 | 1.00 35.91 | AAAA |
| MOTA | 2799 | CB | THR | 350 | 23.421 | 57.615 | 65.952 | 1.00 45.03 | AAAA |
| ATOM | 2800 | OG1 | | 350 | 24.382 | 55.586 | | 1.00 49.48 | AAAA |
| MOTA | 2801 | CG2 | | 350 | 25.821 | 55.267 | 64.330 | 1.00 30.63 | AAAA |
| MOTA | 2802 | C | THR | 350 | 25.535 | 54.709 | 63.274 | 1.00 26.62 | AAAA |
| MOTA | 2803 | 0 | THR | 350 | 26.644 | 54.740 | 65.225 | 1.00 29.07 | AAAA |
| MOTA | 2804 | N | LEU | | 27.271 | 53.461 | | 1.00 24.59 | AAAA |
| MOTA | 2805 | CA | LEU | 351 351 | 28.584 | 53.367 | 65.757 | 1.00 29.91 | AAAA |
| MOTA | 2806 | CB | LEU | 351 | 29.591 | 52.327 | 65.267 | 1.00 39.62 | AAAA |
| ATOM | 2807 | CG | LEU | 351 | 30.887 | 52.467 | 66.039 | 1.00 37.09 | AAAA |
| ATOM | 2808 | | LEU LEU | 351 | 29.024 | 50.935 | 65.415 | 1.00 54.03 | AAAA |
| MOTA | 2809 | | LEU | 351 | 26.314 | 52.336 | 65.377 | 1.00 29.71 | AAAA |
| ATOM | 2810 | C | LEU | 351 | 26.130 | 51.364 | 64.641 | 1.00 30.53 | AAAA |
| MOTA | 2811 | 0 | LYS | 352 | 25.697 | 52.481 | 66.543 | 1.00 28.64 | AAAA |
| MOTA | 2812 | N | LYS | 352 | 24.763 | 51.479 | 67.061 | 1.00 32.72 | AAAA |
| MOTA | 2813 | CA | LYS | 352 | 24.913 | 51.381 | 68.581 | 1.00 27.37 | AAAA |
| ATOM | 2814 | CB CG | LYS | 352 | 26.230 | 50.787 | 69.034 | 1.00 43.48 | AAAA |
| ATOM | 2815 | CD | LYS | 352 | 26.536 | 51.068 | 70.504 | 1.00 46.77 | AAAA |
| ATOM | 2816 2817 | CE | LYS | 352 | 25.484 | 50.538 | 71.451 | 1.00 51.52 | AAAA |
| MOTA | | NZ | LYS | 352 | 25.850 | 50.859 | 72.866 | 1.00 62.08 | АААА |
| MO A | 2818 2819 | C | LYS | 352 | 23.330 | 51.856 | 66.731 | 1.00 32.49 | AAAA |
| MO'. K | 2820 | 0 | LYS | 352 | 22.953 | 53.010 | 66.882 | 1.00 31.90 | AAAA |
| A 1 OM | 2821 | N | ASP | 353 | 22.525 | 50.916 | 66.244 | 1.00 31.44 | AAAA |
| ATOM | 2822 | CA | ASP | 353 | 21.136 | 51.286 | 66.012 | 1.00 26.50 | AAAA |
| ATOM | 2823 | CB | ASP | 353 | 20.543 | 50.635 | 64.746 | 1.00 50.09 | AAAA |
| ATOM | 2824 | CG | ASP | 353 | 20.880 | 49.176 | 64.604 | 1.00 52.79 | AAAA |
| MOTA | 2825 | | ASP | 353 | 21.980 | 48.861 | 64.109 | 1.00 58.55 | АААА |
| MOTA | | | ASP | 353 | 20.040 | 48.339 | 64.984 | 1.00 73.19 | AAAA |
| ATOM | 2826 | | | 353 | 20.328 | 50.930 | 67.257 | 1.00 26.41 | AAAA |
| MOTA | 2827 2828 | CO | ASP ASP | 353 | 20.806 | 50.214 | 68.136 | 1.00 25.73 | AAAA |
| ATOM | 2829 | | PRO | 354 | 19.118 | 51.481 | 67.385 | 1.00 30.12 | AAAA |
| MOTA | | Й | | | 18.428 | 52.429 | 66.495 | 1.00 35.38 | AAAA |
| MOTA | 2830 | CD | PRO | 354 354 | 18.276 | 51.190 | 68.547 | 1.00 34.02 | AAAA |
| MOTA | 2831 | CA | PRO | 354 354 | 17.091 | 52.129 | 68.340 | 1.00 32.25 | AAAA |
| ATOM | 2832 | CB | PRO | 354 354 | 16.974 | 52.139 | 66.833 | 1.00 44.48 | AAAA |
| ATOM | 2833 | CG | PRO | | 17.838 | 49.736 | | 1.00 34.00 | AAAA |
| ATOM | 2834 | C | PRO | 354 | 17.829 | 49.111 | | 1.00 28.28 | AAA |
| ATOM | 2835 | 0 | PRO | 354 | 17.484 | 49.190 | | | TAAA |
| ATCM | 2836 | И | TRP | 355 | 17.010 | 47.818 | | | AAA |
| ATOM | 2837 | CA | TRP | 355 | 16.653 | 47.363 | | | AAAI |
| ATOM | 2838 | CB | TRP | 355 | 10.000 | - ; . 5 0 5 | | = | |

| ATOM | 2839 | CG | TRP | 355 | 17.844 | 46.946 | 71.832 | 1.00 49.97 | AAAA |
|--------------|--------------|----------|------------|------------|-----------------|------------------|------------------|--------------------------|--------------|
| MOTA | 2840 | CDZ | TRP | 355 | 18.364 | 45.622 | 71.905 | 1.00 46.60 | AAAA |
| ATOM | 2841 | _ | TRP | 355 | 19.567 | 45.682 | 72.639 | 1.00 54.73 | AAAA |
| ATOM | 2842 | | TEP | 355 | 17.931 | 44.386 | 71.419 | 1.00 46.90 | AAAA |
| MOTA | 2843 | CDI | | 355 | 18.723 | 47.746 | 72.507 | 1.00 56.10 | AAAA |
| | 2844 | NE1 | | 355 | 19.765 | 46.991 | 72.997 | 1.00 56.07 | AAAA |
| ATOM | 2845 | CZ2 | | 355 | 20.340 | 44.552 | 72.897 | 1.00 55.25 | AAAA |
| MOTA | | CZ3 | | 355 | 18.696 | 43.267 | 71.674 | 1.00 50.74 | AAAA |
| MOTA | 2846 | CH2 | TRP | 355 | 19.887 | 43.356 | 72.405 | 1.00 50.68 | AAAA |
| MOTA | 2847 | Cus | TRP | 355 | 15.789 | 47.712 | 68.776 | 1.00 33.12 | AAAA |
| ATOM | 2848 | 0 | TRP | 355 - | 15.096 | 48.705 | 68.550 | 1.00 29.41 | AAAA |
| ATOM | 2849 2850 | N | ARG | 356 | 15.547 | 46.508 | 68.263 | 1.00 23.90 | AAAA |
| ATOM | 2851 | CA | ARG | 356 | 14.413 | 46.237 | 67.387 | 1.00 23.96 | AAAA |
| MOTA | 2852 | CB | ARG | 356 | 14.892 | 46.096 | 65.935 | 1.00 22.66 | AAAA |
| MOTA | 2853 | CG | ARG | 356 | 15.505 | 47.385 | 65.393 | 1.00 29.06 | AAAA |
| MOTA | 2854 | CD | ARG | 356 | 16.291 | 47.212 | 64.108 | 1.00 28.92 | AAAA |
| MOTA | 2855 | NE | ARG | 356 | 16.833 | 48.503 | 63.686 | 1.00 24.73 | AAAA |
| MOTA MOTA | 2856 | cz | ARG | 356 | 17.733 | 48.668 | 62.724 | 1.00 23.57 | AAAA |
| ATOM | 2857 | NH1 | ARG | 356 | 18.209 | 47.616 | 62.066 | 1.00 22.15 | AAAA |
| ATOM | 2858 | | ARG | 356 | 18.153 | 49.891 | 62.418 | 1.00 22.69 | AAAA |
| ATOM | 2859 | C | ARG | 356 | 13.781 | 44.944 | 67.878 | 1.00 24.89 | AAAA |
| ATOM | 2860 | Õ | ARG | 356 | 13.785 | 43.925 | 67.189 | 1.00 22.25 | AAAA |
| ATOM | 2861 | Ŋ | GLY | 357 | 13.231 | 44:993 | 69.065 | 1.00 23.91 | AAAA |
| ATOM | 2862 | CA | GLY | 357 | 12.631 | 43.805 | 69.657 | 1.00 26.72 | AAAA |
| ATOM | 2863 | C | GLY | 357 | 11.138 | 43.671 | 69.465 | 1.00 26.90 | AAAA |
| ATOM | 2864 | Ö | GLY | 357 | 10.536 | 44.330 | 68.619 | 1.00 29.87 | AAAA |
| ATOM | 2865 | N | GLY | 358 | 10.544 | 42.797 | 70.265 | 1.00 28.22 | AAAA |
| ATOM | 2866 | CA | GLY | 358 | 9.118 | 42.561 | 70.188 | 1.00 30.96 | AAAA |
| MOTA | 2867 | С | GLY | 358 | 8.800 | 41.274 | 70.920 | 1.00 30.03 | AAAA |
| ATOM | 2868 | 0 | GLY | 358 | 9.626 | 40.757 | 71.663 | 1.00 24.03 | AAAA |
| ATOM | 2869 | N | GLU | 359 | 7.601 | 40.747 | 70.715 | 1.00 28.34 | AAAA |
| ATOM | 2870 | CA | GLU | 359 | 7.218 | 39.509 | 71.366 | 1.00 24.37 | AAAA |
| MOTA | 2871 | CB | GLU | 359 | 5.699 | 39.372 | 71.375 | 1.00 32.52 | AAAA |
| MOTA | 2872 | ,CG | GLU | 359 | 4.981 | 40:327 | 72.299 | 1.00 45.44 | AAAA |
| ATOM | 2873 | CD | GLU | 359 | 3.472 | 40.250 | 72.132 | 1.00 50.43 | AAAA |
| ATOM | 2874 | | GLU | 359 | 2.924 | 39.125 | 72.151 | 1.00 42.92 | AAAA |
| MOTA | 2875 | | GLU | 359 | 2.839 | 41.316 | 71.987 | 1.00 40.72 | AAAA AAAA |
| MOTA | 2876 | С | GLU | 359 | 7.804 | 38.323 | 70.628 | 1.00 27.35 1.00 22.94 | AAAA |
| MOTA | 2877 | 0 | GLU | 359 | 8.138 | 38.415 | 69.449 | 1.00 22.94 | AAAA |
| ATOM | 2878 | N | VAL | 360 | 7.944 | 37.208 | 71.325 70.672 | 1.00 13.08 | AAAA |
| MOTA | 2879 | CA | VAL | 360 | 8.441 | 36.017 35.188 | 71.621 | 1.00 26.71 | AAAA |
| ATOM | 2880 | СВ | VAL | 360 | 9.300 9.783 | 33.100 | 70.912 | 1.00 20.71 | AAAA |
| MOTA | 2881 | | AAL | 360 | | 36.038 | 72.113 | 1.00 25.79 | AAAA |
| ATOM | 2882 | | VAL | 360 | 10.486 7.228 | 35.202 | 70.197 | 1.00 25.51 | AAAA |
| MOTA | 2883 | C | VAL | 360 | 6.442 | 34.700 | 71.01 | 1.00 19.75 | AAAA |
| ATOM | 2884 | 0 | VAL | 360 | 7.065 | 35.094 | 68.873 | 1.00 18.48 | AAAA |
| ATOM | 2885 | N | ARG | 361 | 5.947 | 34.337 | 68.3C` | 1.00 22.01 | AAAA |
| ATOM | 2886 | CA | ARG | 361 | 5.988 | 34.389 | 66.772 | 1.00 19.31 | AAAA |
| ATOM | 2887 | CB | ARG | 361 361 | 5.446 | 35.671 | 66.204 | 1.00 30.86 | AAAA |
| MOTA | 2888 | CG | ARG | 361 | 5.735 | 35.730 | 64.723 | 1.00 37.95 | AAAA |
| MOTA | 2889 | CD | ARG | 361 | 7.111 | 36.148 | 64.460 | 1.00 30.73 | AAAA |
| MOTA | 2890 | NE | ARG ARG | 361 | 7.616 | 36.275 | 63.242 | 1.00 22.89 | AAAA |
| MOTA | 2891 | CZ | ARG | 361 | 6.851 | 36.006 | | 1.00 19.02 | AAAA |
| MOTA | 2892 | | ARG | 361 | 8.861 | 36.704 | 63.081 | 1.00 23.47 | AAAA |
| ATOM | 2893 | | | 361 | 5.897 | 32.879 | 68.714 | 1.00 26.11 | AAAA |
| ATOM | 2894 | 0 | ARG | 361 | 6.926 | 32.255 | 68.968 | 1.00 21.79 | AAAA |
| ATOM | 2895 | 0 | ARG LYS | 362 | 4.681 | 32.338 | 68.763 | 1.00 24.89 | AAAA |
| ATOM | 2896 | 11 11 | LYS | 362 | 4.479 | 30.938 | 69.125 | 1.00 28.63 | AAAA |
| ATOM | 2897 | CR | | 362 | 2.981 | 30.570 | 69.070 | 1.00 22.91 | AAAA |
| ATOM | 2898 | CB CG | LYS LYS | 362 | 2.145 | 31.200 | 70.168 | 1.00 50.86 | AAAA |
| ATOM | 2399 | CD | LYS | 362 | 2.290 | 32.715 | 70:157 | 1.00 57.51 | AAAA |
| ATOM | 2900 | CE | LYS | 362 | 1.923 | 33.278 | 68.799 | 1.00 50.87 | AAAA |
| ATOM | 2901 2902 | NZ | LYS | 362 | 2.307 | 34.683 | 68.711 | 1.00 22.99 | AAAA |
| ATCM | | C | LYS | 362 | 5.269 | 30.014 | 68.202 | 1.00 16.77 | AAAA |
| ATCM | 2903 2904 | 0 | LYS | 362 | 5.808 | 29.007 | 68.647 | 1.00 22.90 | AAAA |
| ATOM | ムブリゼ | ~ | | | | · | _ | | |

| ATOM | 2905 | N | GLU | 363 | 5.311 | 30.355 | 66.913 | 1.00 25.24 | AAAA |
|--------------|----------------|---------|-----|------------|------------------|------------------|------------------|--------------------------|---------------|
| ATOM | 2906 | CA | GLU | 363 | 6.055 | 29.577 | 65.910 | 1.00 26.29 | AAAA |
| ATOM | 2907 | CB | GLU | 363 | 6.207 | 30.342 | 64.608 | 1.00 33.50 | AAAA |
| ATOM | 2908 | ĊĠ | GLU | 363 | 4.999 | 30.639 | 63.824 | 1.00 48.73 | ሕ ል ሕሕ |
| ATOM | 2909 | CD | GLU | 363 | 5.368 | 31.494 | 62.638 | 1.00 42.01 | AAAA |
| ATOM - | 2910 | OE1 | GLU | 363 | 6.299 | 31.087 | 61.895 | 1.00 28.50 | AAAA |
| ATOM . | | CE2 | GLU | 363 | 4.738 | 32.558 | 62.461 | 1.00 44.91 | AAAA |
| ATOM | 2912 | c | GLU | 363 | 7.481 | 29.326 | 66.349 | 1.00 19.00 | ÁAAÁ |
| ATOM | 2913 | ō | GLU | 363 | 8.011 | 28.218 | 66.226 | 1.00 18.66 | AAAA |
| ATOM | 2914 | 23 | VAL | 364 | 8.121 | 30.399 | 66.790 | 1.00 20.69 | AAAA |
| ATOM | 2915 | CA | VAL | 364 | 9.501 | 30.303 | 67.219 | 1.00 23.13 | AAAA |
| ATOM | 2916 | C3 | VAL | 364 | 10.096 | 31.681 | 67.510 | 1.00 16.98 | AAAA |
| ATOM | 2917 | | VAL | 364 | 11.515 | 31.513 | 68.010- | | AAAA |
| ATOM | 2918 | | VAL | 364 | 10.082 | 32.548 | 66.242 | 1.00 23.99 | AAAA |
| ATOM | 2919 | c | VAL | 364 | 9.625 | 29.415 | 68.448 | 1.00 19.28 | AAAA |
| MOTA | 2920 | ō | VAL | 364 | 10.507 | 28.548 | 68.510 | 1.00 20.17 | AAAA - |
| ATOM | 2921 | N | LYS | 365 | 8.735 | 29.600 | 69.417 | 1.00 21.11 | AAAA |
| ATOM | 2922 | CA | LYS | 365 | 8.780 | 28.768 | 70.612 | 1.00 18.15 | AAAA |
| ATOM | 2923 | CB | LYS | 365 | 7.711 | 29.210 | 71.626 | 1.00 25.22 | AAAA |
| ATOM | 2924 | CG | LYS | 365 | 7.921 | 30.611 | 72.167 | 1.00 32.99 | AAAA |
| ATOM | 2925 | CD | LYS | 365 | 6.901 | 30.949 | 73.253 | 1.00 36.09 | āAāā |
| ATOM | 2926 | CE | LYS | 365 | 7.121 | 32.357 | 73.790 | 1.00 28.99 | AAAA |
| ATOM | 2927 | NZ | LYS | 365 | 6.178 | 32.736 | 74.882 | 1.00 38.98 | AAAA |
| ATOM | 2928 | C | LYS | 365 | 8.574 | 27.305 | 70.236 | 1.00 19.49 | AAAA |
| ATOM | 2929 | 0 | LYS | 365 | 9.255 | 26.417 | 70.758 | 1.00 22.04 | AAAA |
| ATOM | 2930 | N | ASP | 366 | 7.635 | 27.048 | 69.327 | 1.00 22.45 | AAAA |
| ATOM | 2931 | CA | ASP | 366 | 7.386 | 25.669 | 68.915 | 1.00 22.62 | AAAA |
| ATOM | 2932 | CB | ASP | 366 | 6.173 | 25.574 | 67.967 | 1.00 21.69 | AAAA |
| ATOM | 2933 | CG | ASP | 366 | 4.870 | 25.987 | 68.634 | 1.00 27.75 | AAAA |
| MOTA | 2934 | 0D1 | ASP | 366 | 4.763 | 25.890 | 69.881 | 1.00 31.01 | AAAA |
| MOTA | 2935 | CD2 | ASP | 366 | 3.938 | 26.382 | 67.907 | 1.00 33.20 | AAAA |
| ATOM | 2936 | C | ASP | 366 | 8.606 | 25.034 | 68.237 | 1.00 24.53 | AAAA |
| ATOM | 2937 | 0 | ASP | 366 | 8.924 | 23.871 | 68.480 | 1.00 21.13 | AAAA |
| ATOM | 2938 | 31 | THR | 367 | 9.281 | 25.787 | 67.380 | 1.00 26.19 | AAAA |
| MOTA | 2939 | CA | THR | 367 | 10.462 | 25.252 | 66.694 | 1.00 21.68 | AAAA |
| MOTA | 2940 | CB | THR | 367 | 11.035 | 26.301 | 65.742 | 1.00 14.56 | AAAA |
| MOTA | 2941 | 0G1 | THR | 367 | 10.085 | 26.545 | 64.697 | 1.00 21.76 | AAAA |
| MOTA | 2942 | CG2 | THR | 367 | 12.340 | 25.825 | 65.138 | 1.00 19.83 | AAAA |
| MOTA | 2943 | Ç | THR | 367 | 11.523 | 24.822 | 67.710 | 1.00 19.02 1.00 21.79 | AAAA AAAA |
| MOTA | . 2944 | 0 | THR | 367 | 12.071 | 23.717 | 67.625 | 1.00 21.79 | AAAA |
| MOTA | 2945 | H | LEU | 368 | 11.802 | 25.684 | 68.683 69.700 | 1.00 18.42 | AAAA |
| MOTA | 2946 | CA | LEU | 368 | 12.797 | 25.348 | 70.560 | 1.00 21.02 | AAAA |
| MOTA | 2947 | CB | LEU | 368 | 13.148 | 26.569 27.518 | 69.959 | 1.00 17.34 | AAAA |
| MOTA | 2948 | CG. | LEU | 368 | 14.206 | 26.758 | 69.817 | 1.00 17.43 | AAAA |
| ATOM | 2949 | | LEU | 368 | 15.525 13.756 | 28.041 | 68.593 | 1.00 19.49 | AAAA |
| ATOM | 2950 | D2 | | 368 368 | 12.361 | 24.189 | 70.589 | 1.00 23.17 | AAAA |
| MOTA | 2951 | ÷ | LEU | 368 | 13.203 | 23.420 | 71.052 | 1.00 24.81 | AAAA |
| ATOM | 2952 | er M | LEU | 369 | 11.059 | 24.055 | 70.839 | 1.00 23.97 | AAAA |
| MOTA | 2953 2954 | И СА | GLU | 369 | 10.597 | 22.929 | 71.653 | 1.00 19.36 | AAAA |
| ATOM | 2955 | CE | GLU | 369 | 9.127 | 23.113 | 72.063 | 1.00 21.81 | AAAA |
| ATOM | 2956 | CG | GLU | 369 | 8.913 | 24.225 | 73.100 | 1.00 40.15 | AAAA |
| ATOM ATOM | 2957 | CD | GLU | 369 | 7.450 | 24.416 | 73.487 | 1.00 49.38 | AAAA |
| ATOM | 2958 | DE1 | | 369 | 6.806 | 23.429 | 73.905 | 1.00 43.26 | AAAA |
| ATOM | 2959 | | GLU | 369 | 6.948 | 25.558 | 73.382 | 1.00 57.31 | AAAA |
| | 2960 | C . | GLU | 369 | 10.778 | 21.623 | 70.859 | 1.00 24.29 | AAAA |
| ATOM | 2961 | | GLU | 369 | 11.172 | 20.605 | 71.420 | 1.00 25.96 | AAAA |
| ATOM | 2962 | N. | LYS | 370 | 10.488 | 21.643 | 69.560 | 1.00 22.98 | AAAA |
| ATOM | 2963 | CA. | LYS | 370 | 10.665 | 20.437 | 68.746 | 1.00 23.19 | AAAA |
| ATOM | 2964 | CB | LYS | 370 | 10.051 | 20.596 | 67.347 | 1.00 26.83 | AAAA |
| atom atom | 2965 | CG | LYS | 370 | 8.537 | 20.461 | 67.287 | 1.00 36.68 | AAAA |
| ATOM | 2966 | CD | LYS | 370 | 8.056 | 20.431 | 65.832 | 1.00 39.85 | AAAA |
| ATOM | 2967 | CE | LYS | 370 | 6.567 | 20.105 | 65.740 | 1.00 56.23 | aaaa |
| ATOM | 2968 | :IZ | LYS | 370 | 6.082 | 19.996 | 64.326 | 1.00 56.10 | AAAA |
| ATOM | 2969 | c | LYS | 370 | 12.148 | 20.123 | 68.602 | 1.00 31.63 | AAAA |
| ATOM | 2970 | 5 | LYS | 370 | 12.549 | 18.958 | 68.587 | 1.00 36.88 | AAAÁ |
| | · - | - | | | | | - | | |

| ATOM | 2971 | N | ALA | 371 | 12.961 | 21.170 | 68.491 | 1.00 26.25 | AAAA |
|------------------|------|-----|------|----------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 2972 | CA | ALA | 371 | 14.407 | 21.009 | 68.360 | 1.00 27.33 | AAAA |
| ATOM | 2973 | СВ | ALA | 371 | 15.079 | 22.370 | 68.188 | 1.00 23.70 | AAAA |
| ATOM | 2974 | c | ALA | 371 | 14.989 | 20.308 | 69.581 | 1.00 26.74 | AAAA |
| ATOM | 2975 | Ö | ALA' | 371 | 15.892 | 19.482 | 69.452 | 1.00 29.52 | AAAA |
| ATOM | 2976 | Ŋ | ALA | 372 | 14.484 | 20.652 | 70.764 | 1.00 24.83 | AAAA |
| ATOM | 2977 | CA | ALA | 372 | 14.959 | 20.055 | 72.012 | 1.00 34.24 | AAAA |
| ATOM | 2978 | CB | ALA | 372 | 14.305 | 20.750 | 73.214 | 1.00 37.17 | AAAA |
| ATOM | 2979 | С | ALA | .372 | 14.663 | 18.564 | 72.061 | 1.00 45.62 | AAAA |
| ATOM | 2980 | 0 | ALA | 372 | 15.563 | 17.741 | 72.280 | 1.00 35.52 | AAAA AAAA |
| MOTA | 2981 | N | ALA | 373 | 13.394 | 18.216 | 71.869 | 1.00 44:50 | • |
| MOTA | 2982 | CA | ALA | 373 | 13.004 | 16.813 | 71.892 | 1.00 49.88 | AAAA AAAA |
| MOTA | 2983 | CB | ALA | 373 | 11.506 | 16.681 | 71.628 | 1.00 49.32 1.00 44.64 | AAAA |
| ATOM | 2984 | С | ALA | 373 | 13.807 | 16.072 | 70.825 | 1.00 58.19 | AAAA |
| MOTA | 2985 | 0 | ALA | 373 | 14.669 | 15.250 | 71.201 69.626 | 1.00 41.63 | AAAA |
| MOTA | 2986 | | ALA | 373 | 13.591 | 16.337 | 49.242 | 1.00 13.03 | SOLV |
| HETATM | 2987 | OH2 | | 1 | 36.368 23.107 | 43.907 30.584 | 59.802 | 1.00 11.42 | SOLV |
| HETATM | 2988 | | TAW | 2 | 20.594 | 33.744 | 61.457 | 1.00 14.73 | SOLV |
| HETATM | | | WAT | 3 4 | 31.359 | 16.551 | 51.590 | 1.00 19.84 | SOLV |
| HETATM | 2990 | OH2 | | 5 | 30.389 | 18.140 | 45.769 | 1.00 19.94 | SOLV |
| HETATM | 2991 | | TAW | 6 | 16.925 | 41.748 | 56.551 | 1.00 13.33 | SOLV |
| HETATM | 2992 | OH2 | | 7 | 28.448 | 16.084 | 62.316 | 1.00 14.08 | SOLV |
| HETATM HETATM | 2004 | | WAT | · 8 | 40.375 | 38.476 | 55.678 | 1.00 19.10 | SOLV |
| HETATM | | | WAT | 9 | 18.455 | 29.667 | 54.797 | 1.00 18.81 | SOLV |
| HETATM | 2995 | | WAT | 10 | 26.305 | 18.390 | 59.507 | 1.00 16.65 | SOLV |
| HETATM | 2997 | | WAT | 11 | 50.145 | 32.063 | 58.142 | 1.00 16.53 | SOLV |
| HETATM | 2998 | | TAW | 12 | 45.935 | 30.996 | 40.672 | 1.00 25.08 | SOLV |
| HETATM | 2999 | | WAT | 13 | 26.358 | 43.110 | 74.179 | 1.00 22.91 | SOLV |
| HETATM | | | WAT | 14 | 48.727 | 24.720 | 56.917 | 1.00 25.49 | SOLV |
| HETATM | | | WAT | 15 | 30.244 | 18.663 | 50.165 | 1.00 25.78 | SOLV |
| HETATM | | OH2 | TAW | 16 | 10.615 | 28.799 | 63.631 | 1.00 22.40 | SOLV |
| HETATM | | OH2 | WAT | 17 | 18.401 | 20.018 | 62.704 | 1.00 21.46 | SOLV |
| HETATM | 3004 | OH2 | WAT | 18 | 22.195 | 47.791 | 60.896 | 1.00 26.19 1.00 20.38 | SOLV |
| HETATM | 3005 | | TAW | 19 | 3.278 | 32.141 | 65.350 | 1.00 20.38 | SOLV |
| HETATM | | | TAW | 20 | 23.643 | 22.897 | 59.512 48.818 | 1.00 21.27 | SOLV. |
| HETATM | | | TAW | . 21 | 50.287 44.725 | 23.101 34.256 | 46.541 | 1.00 18.74 | SOLV |
| HETATM | | | WAT | 22 | 8.346 | 30.527 | 49.922 | 1.00 22.33 | SOLV |
| HETATM | | | TAW | 23 | 39.855 | 33.795 | 67.390 | 1.00 20.43 | SOLV |
| HETATM | | | TAW | 24 25 | 7.827 | 32.763 | 57.779 | 1.00 19.24 | SOLV |
| HETATM | | | WAT | 26 | 45.388 | 34.567 | 36.246 | 1.00 20.86 | SOLV |
| HETATM HETATM | 3012 | | WAT | 27 | 47.636 | 32.244 | 33.388 | 1.00 20.41 | SOLV |
| HETATM | 3013 | | WAT | 28 | 32.514 | 35.684 | 41.278 | 1.00 24.76 | SOLV |
| HETATM | 3015 | | WAT | | 26.188 | 15.341 | 61.913 | 1.00 19.63 | SOLV |
| HETATM | 3016 | | TAW | 30 | 14.957 | 43.169 | 56.333 | 1.00 23.80 | SOLV |
| HETATM | 3017 | | WAT | 31 | 24.483 | 43.556 | 55.704 | 1.00 27.25 | SOLV |
| HETATM | 3018 | | TAW | 32 | 41.141 | 16.376 | 48.456 | 1.00 25.99 | SOLV |
| HETATM | | | WAT | 33 | 23.104 | 17.625 | 54.086 | 1.00 26.37 | SOLV |
| HETATM | 3020 | | WAT | 34 | 51.301 | 28.602 | 57.694 | 1.00 32.78 | SOLV |
| HETATM | 3021 | OH2 | WAT | 35 | 51.376 | 29.469 | 53.156 | 1.00 24.27 | SOLV SOLV |
| HETATM | 3022 | OH2 | WAT | 36 | 12.518 | 22.131 | 49.816 | 1.00 23.60 | SOLV |
| HETATM | 3023 | OH2 | WAT | 37 | 6.521 | 27.442 | 50.861 | 1.00 25.87 1.00 19.87 | SOLV |
| HETATM | 3024 | OH2 | WAT | 38 | 30.390 | 33.757 | 34.190 | 1.00 19.87 | SOLV |
| HETATM | 3025 | | WAT | 39 | 8.328 | 29.586 | 62.062 30.724 | 1.00 32.61 | SOLV |
| HETATM | 3026 | | TAW | 40 | 30.180 | 24.235 | | 1.00 27.52 | SOLV |
| HETATM | 3027 | | TAW | 41 | 44.521 | 30.663 | 38.395 41.186 | 1.00 27.32 | SOLV |
| HETATM | 3028 | | TAW | 42 | 30.981 | 18.043 | 73.830 | 1.00 29.36 | SOLV |
| HETATM | 3029 | | TAW | 43 | 14.632 | 37.127 | 72.230 | 1.00 21.87 | |
| HETATM | 3030 | | TAW | 44 | 39.332 | 25.953 37.592 | 51.896 | 1.00 39.62 | SOLV |
| HETATM | 3031 | | TAW | 45 | 7.597 15.027 | 18.079 | 54.827 | 1.00 26.65 | SOLV |
| HETATM | 3032 | | WAT | 46 | 11.076 | 45.493 | 66.435 | 1.00 38.18 | SOLV |
| HETATM | 3033 | | WAT | 47 | 42.124 | 18.055 | 37.233 | 1.00 28.62 | SOLV |
| HETATM | 3034 | | TAW | 48 49 | 48.736 | 25.764 | 64.149 | 1.00 31.88 | SOLV |
| HETATM | | | WAT | | 50.383 | 27.254 | 54.972 | 1.00 24.36 | SOLV |
| HETATM | 2030 | UMZ | WAT | J (| 20.00 | | - | | |

| | | | | | 40 (50 | 36 035 | 68.226 | 1.00 33.89 | SOLV |
|---|--|--|--|---|---|--|--|--|--|
| HETATM | | CH2 | | 51 | 48.659 | 36.025 | | | |
| HETATM | 3038 | OH2 | TAW | 52 | 36.998 | 27.228 | 71.440 | 1.00 21.03 | SOLV |
| HETATM | | OH2 | WAT | 53 | 41.303 | 16.309 | 55.307 | 1.00 32.23 | SOLV |
| HETATM | | OH2 | | 54 | 33.242 | 39.524 | 49.454 | 1.00 29.77 | SOLV |
| | | | | | 45.004 | 25.973 | 35.031 | 1.00 21.59 | SOLV |
| HETATM | | OH2 | | 55 | | | | | - |
| HETATM | 3042 | OH2 | WAT | 56 | 19.039 | 25.829 | 45.793 | 1.00 33.48 | SOLV |
| HETATM | | OH2 | ጥልመ | 57 | 17.922 | 35.542 | 50.154 | 1.00 37.51 | SOLV |
| | | CH2 | | 58 | 10.409 | 26.864 | 73.166 | 1.00 26.54 | SOLV |
| HETATM | | | | | | | 59.408 | 1.00 20.83 | SOLV |
| HETATM | 3045 | OH2 | WAT | 59 | 11.835 | 22.805 | | | |
| HETATM | 3046 | OH2 | TAW | 60 | 18.254 | 48.699 | 53.224 | 1.00 28.41 | SOLV |
| HETATM | | OH2 | UAT | 61 | 10.426 | 26.647 | 60.447 | 1.00 32.72 | SOLV |
| | | OH2 | | 62 | 21.304 | 55.086 | 63.510 | 1.00 28.84 | SOLV |
| HETATM | | | | | | 51.211 | 45.469 | 1.00 32.48 | SOLV |
| HETATM | | OH2 | | 63 | 32.532 | | | | SOLV |
| HETATM | 3050 | OH2 | TAW | 64 | 22.658 | 61.079 | 57.420 | 1.00 27.32 | |
| HETATM | | OH2 | TAW | 65 | 16.734 | 24.334 | 74.721 | 1.00 27.44 | SOLV |
| | | OH2 | | 66 | 32.758 | 37.824 | 54.391 | 1.00 25.07 | SOLV |
| HETATM | | | | | 11.142 | 25.859 | 49.706 | 1.00 29.66 | SOLV |
| HETATM | | OH2 | WAT | 67 | | | | | SOLV |
| HETATM | 3054 | OH2 | WAT | 68 | 24.192 | 15.261 | 53.236 | 1.00 30.21 | |
| HETATM | | OH2 | TAV | 69 | 19.816 | 17.916 | 66.357 | 1.00 30.50 | SOLV |
| HETATM | | OH2 | | 70 | 50.347 | 23.975 | 53.197 | 1.00 28.08 | SOLV |
| | | | | | 50.258 | 30.918 | 51:113 | 1.00 20.19 | SOLV |
| HETATM | | OH2 | | 71 | | | | | SOLV |
| HETATM | 3058 | OH2 | WAT | 72 | 21.047 | 17.624 | 68.693 | 1.00 41.23 | |
| HETATM | | OH2 | VAT | 73 | 26.782 | 33.756 | 49.995 | 1.00 25.80 | SOLV |
| | | OH2 | | 74 | 12.570 | 43.844 | 64.441 | 1.00 31.03 | SOLV |
| HETATM | | | | | 35.555 | 41.287 | 50.852 | 1.00 24.03 | SOLV |
| HETATM | | OH2 | | 75 | _ | | | | SOLV |
| HETATM | 3062 | OH2 | WAT | 76 | 27.764 | 18.231 | 61.827 | 1.00 18.28 | |
| HETATM | | OH2 | WAT | 77 | 26.715 | 29.236 | 38.391 | 1.00 23.18 | SOLV |
| HETATM | | OH2 | | 78 | 21.461 | 23.245 | 48.872 | 1.00 23.80 | SOLV |
| | | | | | 49.246 | 28.263 | 65.477 | 1.00 21,52 | SOLV |
| HETATM | | OH2 | | 79 | | | | | SOLV |
| HETATM | 3066 | OH2 | WAT | 80 | 31.785 | 13.301 | 69.606 | 1.00 31.11 | |
| HETATM | | OH2 | WAT | 81 | 49.811 | 34.740 | 59.229 | 1.00 31,76 | SOLV |
| HETATM | | | WAT | 82 | 45.670 | 33.188 | 42.470 | 1.00 23.13 | SOLV |
| HETATM | 3000 | | | | 9.408 | 39.751 | 55.872 | 1.00 31.53 | SOLV |
| HETATM | | OH2 | | 83 | | | | 1.00 37.32 | SOLV |
| HETATM | 3070 | OH2 | WAT | 84 . | 35.166 | 35.878 | 29.899 | | |
| HETATM | | OH2 | WAT | 85 | 41.927 | 22.970 | 73.694 | 1.00 44.07 | SOLV |
| HETATM | | | WAT | 86 | 22.125 | 34.577 | 49.199 | 1.00 44.65 | SOLV |
| | | | | 87 | 43.984 | 33.541 | 37.965 | 1.00 24.88 | SOLV |
| HETATM | | | WAT | | | | 56.312 | 1.00 34.85 | SOLV |
| HETATM | 3074 | OH2 | WAT | 88 | 11.997 | 17.962 | | | |
| HETATM | 3075 | OH2 | WAT | 89 | 42.194 | 14.737 | 59.766 | 1.00 25.91 | SOLV |
| HETATM | | | TAW | 90 | 49.313 | 24.200 | 41.684 | 1.00 29.29 | SOLV |
| | | | WAT | 91 | 48.504 | 33.595 | 61.519 | 1.00 30.32 | SOLV |
| HETATM | | | | | 24.773 | 18.356 | 33.365 | 1.00 53.13 | SOLV |
| HETATM | | | MAT | 92 | | | | | SOLV |
| HETATM | 3079 | OH2 | TAW | 93 | 35.160 | 35.656 | 47.470 | 1.00 41.41 | |
| HETATM | | OH2 | WAT | 94 | 44.682 | 36.658 | 39.962 | 1.00 29.24 | SOLV |
| | | | WAT | 95 | 9.576 | 41.033 | 52.549 | 1.00 51.83 | ·SOLV |
| HETATM | | | | | 47.199 | 20.112 | 42.102 | 1.00 40.39 | SOLV |
| HETATM | | | $\mathbf{T}\mathbf{A}W$ | `6 | | | | 1.00 37.03 | SOLV |
| HETATM | 3083 | OH2 | TAW | 7ر ٠ | 49.254 | 26.331 | 59.641 | 1.00 37.03 | 300 |
| HETATM | 3084 | | WAT | • | | | | | 20111 |
| | | OH2 | | - 0 | 26.808 | 37.600 | 38.172 | 1.00 28.74 | SOLV |
| HETAIM | | | | _8 | | | 38.172 | 1.00 28.74 | SOLV SOLV |
| | 3085 | OH2 | TAW | 99 | 40.749 | 14.572 | 38.172 64.635 | 1.00 28.74 1.00 33.42 | SOLV |
| HETATM | 3085 3086 | OH2 OH2 | WAT WAT | 99 100 | 40.749 24.850 | 14.572 44.161 | 38.172 64.635 47.775 | 1.00 28.74 1.00 33.42 1.00 27.89 | SOLV SOLV |
| HETATM | 3085 3086 | OH2 OH2 OH2 | TAW TAW TAW | 99 | 40.749 24.850 34.326 | 14.572 44.161 42.063 | 38.172 64.635 47.775 46.714 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 | SOLV SOLV SOLV |
| HETATM HETATM | 3085 3086 3087 | OH2 OH2 OH2 | TAW TAW TAW | 99 100 101 | 40.749 24.850 | 14.572 44.161 | 38.172 64.635 47.775 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 | SOLV SOLV SOLV |
| HETATM HETATM HETATM | 3085 3086 3087 3088 | OH2 OH2 OH2 OH2 | TAW TAW TAW TAW | 99 100 101 102 | 40.749 24.850 34.326 30.226 | 14.572 44.161 42.063 34.544 | 38.172 64.635 47.775 46.714 52.026 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 | SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 | OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW | 99 100 101 102 103 | 40.749 24.850 34.326 30.226 47.824 | 14.572 44.161 42.063 34.544 39.054 | 38.172 64.635 47.775 46.714 52.026 78.097 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 1.00 52.16 | SOLV SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 3090 | OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW | 99 100 101 102 103 104 | 40.749 24.850 34.326 30.226 47.824 19.665 | 14.572 44.161 42.063 34.544 39.054 18.953 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 1.00 52.16 1.00 51.70 | SOLV SOLV SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 3090 | OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW | 99 100 101 102 103 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 1.00 52.16 1.00 51.70 1.00 23.65 | SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 3090 3091 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 | 40.749 24.850 34.326 30.226 47.824 19.665 | 14.572 44.161 42.063 34.544 39.054 18.953 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 1.00 52.16 1.00 51.70 1.00 23.65 1.00 37.56 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 30.77 1.00 52.16 1.00 51.70 1.00 23.65 | SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM HETATM HETATM HETATM HETATM HETATM HETATM HETATM HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 39.55 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 42.61 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 3095 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 37.56 1.00 46.95 1.00 42.61 1.00 31.59 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 3095 3096 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 42.61 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 3095 3096 3097 | OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 | TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 42.61 1.00 31.59 1.00 49.09 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3096 3097 3098 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 26.174 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 33.692 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 37.56 1.00 46.95 1.00 39.55 1.00 39.55 1.00 42.61 1.00 31.59 1.00 49.09 1.00 36.61 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3096 3097 3098 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 26.174 23.545 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 33.692 20.203 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 37.56 1.00 39.55 1.00 46.95 1.00 31.59 1.00 49.09 1.00 36.61 1.00 24.34 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3090 3091 3092 3093 3094 3095 3096 3097 3098 3099 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 26.174 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 33.692 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 57.697 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 46.95 1.00 37.56 1.00 39.55 1.00 49.09 1.00 36.61 1.00 24.34 1.00 33.65 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3096 3097 3098 3099 3100 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 26.174 23.545 9.083 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 33.692 20.203 42.965 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 57.697 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 46.95 1.00 39.55 1.00 31.59 1.00 36.61 1.00 24.34 1.00 33.65 1.00 33.65 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3095 3099 3100 3101 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.398 26.174 23.545 9.083 8.442 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.073 33.692 20.203 42.965 39.898 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 57.697 64.594 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 46.95 1.00 39.55 1.00 31.59 1.00 36.61 1.00 24.34 1.00 33.65 1.00 33.65 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3095 3099 3100 3101 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.624 51.398 26.174 23.545 9.083 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.591 26.073 33.692 20.203 42.965 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 57.697 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 46.95 1.00 37.56 1.00 39.55 1.00 49.09 1.00 36.61 1.00 24.34 1.00 33.65 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |
| HETATM | 3085 3086 3087 3088 3089 3091 3092 3093 3095 3095 3099 3100 3101 | OH2 | TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW | 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 | 40.749 24.850 34.326 30.226 47.824 19.665 46.857 48.069 15.553 44.026 8.139 50.398 26.174 23.545 9.083 8.442 | 14.572 44.161 42.063 34.544 39.054 18.953 36.525 19.460 56.850 19.119 42.064 36.073 33.692 20.203 42.965 39.898 | 38.172 64.635 47.775 46.714 52.026 78.097 47.438 46.232 67.360 61.838 70.671 65.674 65.779 61.043 33.551 53.001 57.697 64.594 | 1.00 28.74 1.00 33.42 1.00 27.89 1.00 42.22 1.00 52.16 1.00 51.70 1.00 23.65 1.00 46.95 1.00 46.95 1.00 39.55 1.00 31.59 1.00 36.61 1.00 24.34 1.00 33.65 1.00 33.65 | SOLV SOLV SOLV SOLV SOLV SOLV SOLV SOLV |

| HETATM | 2103 | 042 | WAT | 117 | 15.41 | 17 38.438 | 50.473 | 1.00 34.46 | SOLV |
|-----------|--------------|------|----------------------------------|--------|----------|-----------|--------|-------------|--------|
| | | | | | | | | | |
| HETATM | 3104 | OH2 | WAT | 118 | 40.75 | | 29.206 | 1.00 29.12 | SOLV |
| HETATM | 3105 | OH2 | WAT | 119 | 27.71 | 17 18.542 | 46.553 | 1.00 28.17 | SOLV |
| | | | | | | | 56.845 | 1.00 38.56 | SOLV |
| HETATM | 3106 | OH2 | WAT | 120 | 18.61 | | | | |
| HETATM | 3107 | OH2 | WAT | 121 | 43.19 | 8 31.377 | 72.139 | 1.00 26.31 | SOLV |
| | | | | | 44.18 | | 33.802 | 1.00 29.81 | SOLV |
| HETATM | | | TAW | 122 | | | | | |
| HETATM | 3109 | OH2 | WAT | 123 | 50.73 | 6 40.909 | 58.456 | 1.00 32.40 | SOLV |
| | | | | | 31.30 | | 31.742 | 1.00 30.84 | SOLV |
| HETATM | | OHZ | WAT | 124 | | | | | |
| HETATM | 3111 | OH2 | WAT | 125 | 36.89 | 5 21.264 | 34.198 | 1.00 34.67 | SOLV |
| | | | | 126 | 47.47 | | 67.427 | 1.00 34.35 | SOLV |
| HETATM | | | TAW | | | | | | |
| HETATM | 3113 | OH2 | WAT | 127 | . 7.17 | 78 25.936 | 64.063 | 1.00 31.77 | SOLV |
| HETATM | 2114 | OU 2 | WAT | 128 | 36.36 | 66.647 | 54.021 | 1.00 36.88 | SOLV |
| | | | | | | | 30.348 | 1.00 26.61 | SOLV |
| HETATM | 3115 | OH2 | WAT | 129 | 42.48 | | | | |
| HETATM | 3116 | OH2 | TAW | 130 | 8.43 | 34.383 | 50.442 | 1.00 37.45 | SOLV |
| | | | | | 37.64 | | 48.946 | 1.00 37.33 | SOLV |
| HETATM | | | TAW | 131 | | | | | |
| HETATM | 3118 | OH2 | WAT | 132 | 50.27 | 73 41.645 | 63.380 | 1.00 37.33 | SOLV |
| HETATM | | | WAT | 133 | 7.53 | 18 26.633 | 61.571 | 1.00 45.42 | SOLV |
| | | | | | | | | | SOLV |
| METATM | 3120 | OH2 | $\mathbf{T}\mathbf{A}\mathbf{W}$ | 134 | 31.48 | | 72.538 | 1.00 28.02 | |
| HETATM | 3121 | OH2 | TAW | 135 | 41.50 | 16.604 | 58.054 | 1.00 32.78 | SOLV |
| TID TATE | 2122 | | | 136 | 45.89 | | 55.185 | 1.00 43.47 | SOLV |
| HETATM | | | TAW | | | | | | |
| HETATM | 3123 | OH2 | WAT | 137 | 16.30 | 0 33.614 | 49.519 | 1.00 30.37 | SOLV |
| HETATM | | | WAT | | 51.14 | 18 36.946 | 55.148 | 1.00 46.34 | SOLV |
| | | | | | | | | | SOLV |
| HETATM | 3125 | | WAT | 139 | | | 50.892 | 1.00 38.27 | |
| HETATM | 3126 | OH2 | TAW | 140 | 21.60 | 3 54.580 | 68.690 | 1.00 33.10 | SOLV |
| | | | | | 10.19 | | 60.325 | 1.00 30.24 | SOLV |
| MTATAH | | | TAW | 141 | | | | | |
| HETATM | 3128 | OH2 | WAT | 142 | 16.95 | 18.120 | 66.901 | 1.00 40.85 | SCLV |
| HETATM | 2120 | | WAT | 143 | 4.94 | 3 24.912 | 51.199 | 1.00 49.13 | SOLV |
| | | | | | | | | 1.00 30.72 | SOLV |
| HETATM | 3130 | OH2 | TAW | 144 | 10.73 | | 58.177 | | |
| HETATM | | OH2 | TAW | 145 | 30.81 | L5 43.398 | 36.040 | 1.00 42.23 | SOLV |
| | | | | | 21.76 | | 46.695 | 1.00 28.31 | SOLV |
| HETATM | | | WAT | 146 | | | | | |
| HETATM | 3133 | OH2 | WAT | 147 | 51.78 | 38 33.122 | 50.887 | 1.00 26.15 | SOLV |
| HETATM | | | WAT | 148 | 24.53 | 31 44.741 | 72,420 | 1.00 27.99 | SOLV |
| | | | | | | | 60.422 | 1.00 38.20 | · SOLV |
| HETATM | 3135 | OH2 | WAT | 149 | 50.93 | | | | |
| HETATM | 3136 | OH2 | WAT | 150 | 24.86 | 50 47.932 | 61.067 | 1.00 18.89 | SOLV |
| neinii | 2127 | | | 151 | 27.33 | | 35.642 | 1.00 33.58 | SOLV |
| HETATM | 313/ | | TAV! | | | | | | |
| HETATM | 3138 | OH2 | TAW | 152 | 38.68 | 30 35.535 | 35.974 | 1.00 26.89 | SOLV |
| HETATM | 2120 | OH2 | WAT | 153 | 24.44 | 11 16.097 | 33.317 | 1.00 48.33 | SOLV |
| | | | | | 20.34 | | 73.416 | 1.00 36.28 | SOLV |
| HETATM | | OHZ | TAW | 154 | | | | | |
| HETATM | 3141 | OH2 | WAT | 155 | 49.76 | 55 37.948 | 74.801 | 1.00 48.41 | SOLV |
| TIPE MA | 33.40 | | TAW | 156 | 34.32 | 29 31.169 | 47.547 | 1.00 25.33 | SOLV |
| HETATM | 2142 | | | | | | _ | | SOLV |
| HETATM | 3143 | OH2 | TAW | 157 | 43.02 | 28 24.554 | 72.536 | 1.00 41.54 | |
| HETATM | 3144 | OH2 | WAT | 158 | 39.88 | 38 15.082 | 42.035 | 1.00 28.76 | SOLV |
| | | | | | 41.88 | | 73.179 | 1.00 51.03 | SOLV |
| HETATM | | | WAT | 159 | | | | | |
| HETATM | 3146 | OH2 | TAW | 160 | 22.96 | 52 49.969 | 58.518 | 1.00 35.04 | SOLV |
| HETATM | | | TAW | 161 | 14.69 | 96 15.261 | 68.016 | 1.00 55.47 | SOLV |
| | | | | | | | 64.866 | 1.00 42.00 | SOLV |
| HETATM | | QHZ | TAW | 162 | 14.9 | | | | |
| HETATM | 3149 | OH2 | WAT | 163 | 30.60 | 08 49.029 | 52.612 | 1.00 47.32 | . SOLV |
| ********* | 2150 | | TAW | 164 | 52.50 | | 57.612 | 1.00 36.71 | SOLV |
| HETATM | | | | | | | | | SOLV |
| HETATM | 3 151 | OH2 | WAT | 165 | 23.69 | | 77.729 | 1.00 32.22 | |
| HETATM | | OH2 | TAW | 166 | 36.97 | 71 59.046 | 63.272 | 1.00 43.05 | SOLV |
| | | | | | | | 52.876 | 1.00 33.66 | SOLV |
| HETATM | 3153 | OHZ | TAW | 167 | 46.05 | | | | |
| HETATM | 3154 | OH2 | WAT | 168 | 42.78 | 30 49.151 | 58.106 | .1.00 44.63 | SOLV |
| | | | TAW | 169 | 15.10 | 00 44.506 | 72.183 | 1.00 45.43 | SOLV |
| HETATM | | | | | | | | | SOLV |
| HETATM | 3156 | OH2 | WAT | 170 | 31.67 | | | 1.00 34.51 | |
| HETATM | 3157 | | WAT | 171 | 25.33 | 36 45.674 | 45.578 | 1.00 55.85 | SOLV |
| RETAIN | 3131 | | | | | | 49.018 | 1.00 32.73 | SOLV |
| HETATM | | | WAT | 172 | 17.48 | | | | |
| HETATM | | OH2 | WAT | 173 | 26.13 | 12 18.147 | 31.404 | 1.00 49.94 | SOLV |
| | | | | | 45.8 | | 70.985 | 1.00 32.89 | SOLV |
| HETATM | 3700 | | TAW | 174 | | | | | SOLV |
| HETATM | 3161 | CH2 | WAT | 175 | 34.5 | | 33.278 | 1.00 42.20 | |
| | | | WAT | 176 | 16.33 | | 50.466 | 1.00 40.74 | SOLV |
| HETATM | | | | | | | 74.689 | 1.00 38.56 | SOLV |
| HETATM | 3163 | | TAV: | 177 | 31.40 | | | | |
| HETATM | | OH2 | TAW | 178 | 50.9 | 71 27.079 | 67.130 | 1.00 44.49 | SOLV |
| | | | | 179 | 7.9: | | 54.691 | 1.00 42.84 | SOLV |
| HETATM | 2102 | | TAW | | | | | 1.00 35.99 | SOLV |
| HETATM | 3166 | OH2 | TAW | 180 | 33.49 | | 73.612 | | |
| НЕТАТМ | 3167 | | WAT | 181 | 26.0 | 16 19.583 | 44.954 | 1.00 51.31 | SOLV |
| | | | WAT | 182 | 40.1 | | 74.920 | 1.00 43.64 | SOLV |
| | 3168 | mu) | TAL A TT | 1 24 / | 44 U . 1 | 37 17.020 | 12.240 | T | |

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| | 3160 | 053 | WAT | 183 | 10.441 | 42.659 | 62.744 | 1.00 34.51 | SOLV |
|---------------|------|-----|------|-----|--------|--------|------------------|------------|------|
| HETATM | | | TAW | 184 | 2.095 | 34.482 | 65.810 | 1.00 36.49 | SOLV |
| HETATM | | OH2 | _ | 185 | 45.749 | 18.286 | 51.615 | 1.00 28.19 | SOLV |
| HETATM | | | WAT | 186 | 25.771 | 38.332 | 76.707 | 1.00 45.53 | SOLV |
| HETATM | 31/2 | | | 187 | 7.228 | 40.382 | 57.542 | 1.00 48.91 | SOLV |
| HETATM | | | TAW | | 42.972 | 52.824 | 67.739 | 1.00 39.99 | SOLV |
| HETATM | | | TAW | 188 | 20.137 | 13.189 | 73.277 | 1.00 44.91 | SOLV |
| HETATM | | | TAW | 189 | _ | 19.193 | 47.581 | 1.00 52.88 | SOLV |
| HETATM | | | TAW | 190 | 48.945 | 34.547 | 47.665 | 1.00 49.15 | SOLV |
| НЕТАТМ | 3177 | | TAW | 191 | 14.549 | 20.567 | 26.536 | 1.00 42.23 | SOLV |
| HETATM | | | TAW | 192 | 31.765 | | 74.222 | 1.00 32.10 | SOLV |
| METATM | | | WAT | 193 | 9.784 | 39.303 | 52.375 | 1.00 50.98 | SOLV |
| HETATM | | | WAT | 194 | 28.865 | 12.481 | 70.409- | 1.00 52.43 | SOLV |
| HETATM | | | TAW | 195 | 24.030 | 12.804 | 50.698 | 1.00 43.03 | SOLV |
| HETATM | 3182 | | WAT | 196 | 47.209 | 39.536 | 27.306 | 1.00 41.11 | SOLV |
| HETATM | 3183 | | WAT | 197 | 35.618 | 18.114 | 43.853 | 1.00 48.20 | SOLV |
| HETATM | | | TAW | 198 | 23.625 | 48.145 | 54.185 | 1.00 34.99 | SOLV |
| HETATM | | | WAT | 199 | 37.090 | 59.044 | 59.080 | 1.00 34.55 | SOLV |
| HETATM | 3186 | | TAW | 200 | 34.478 | 12.208 | 76.228 | 1.00 33.95 | SOLV |
| HETATM | | | WAT | 201 | 22.142 | 29.583 | 53.973 | 1.00 33.93 | SOLV |
| HETATM | | | TAW | 202 | 13.608 | 42.619 | | 1.00 40.44 | SOLV |
| HETATM | | | TAW | 203 | 42.647 | 18.701 | 72.526 | 1.00 33.84 | SOLV |
| HETATM | | | WAT | 204 | 37.005 | 35.993 | 77.480 | 1.00 34.82 | SOLV |
| HETATM | | | TAW | 205 | 34.154 | 20.512 | 33.327 | 1.00 49.58 | SOLV |
| HETATM | 3192 | | WAT | 206 | 37.264 | 57.546 | 47.642 | 1.00 49.38 | SOLV |
| HETATM | | | WAT | 207 | 17.924 | 35.195 | 79.003 | 1.00 35.37 | SOLV |
| HETATM | | | WAT | 208 | 51.172 | 31.581 | 62.378 | 1.00 39.95 | SOLV |
| HETATM | | | TAU | 209 | 50.503 | 36.726 | 79.224 | 1.00 52.08 | SOLV |
| HETATM | 3196 | | TAW | 210 | 18.382 | 13.162 | 63.852 | 1.00 32.08 | SOLV |
| HETATM | 3197 | | WAT | 211 | 27.245 | 8.351 | 55.199 59.540 | 1.00 39.12 | SOLV |
| HETATM | 3198 | | TAW | 212 | 18.354 | 13.545 | 63.388 | 1.00 36.69 | SOLV |
| HETATM | 3199 | | WAT | 213 | 49.088 | 51.744 | 50.871 | 1.00 30.03 | SOLV |
| HETATM | | | WAT | 214 | 23.251 | 33.160 | 50.651 | 1.00 38.63 | SOLV |
| HETATM | 3201 | | WAT. | 215 | 12.989 | 35.073 | 43.239 | 1.00 37.93 | SOLV |
| HETATM | | | TAN | 216 | 24.414 | 44.460 | 73.117 | 1.00 34.17 | SOLV |
| HETATM | 3203 | | TAW | 217 | 24.690 | 47.590 | 81.360 | | SOLV |
| HETATM | 3204 | | WAT | 218 | 19.844 | 17.949 | 74.247 | 1.00 37.83 | SOLV |
| HETATM | 3205 | | WAT | 219 | 40.169 | 27.215 | 73.171 | 1.00 49.20 | SOLV |
| HETATM | 3206 | | WAT | 220 | 38.737 | 39.516 | | 1.00 45.57 | SOLV |
| HETATM | | | TAW | 221 | 50.628 | 21.408 | 46.879 75.660 | 1.00 43.37 | SOLV |
| HETATM | | | TAW | 222 | 35.436 | 43.288 | 55.285 | 1.00 37.33 | SOLV |
| HETATM | | | TAW | 223 | 34.390 | 16.963 | 34.475 | 1.00 35.10 | SOLV |
| HETATM | 3210 | | TAW | 224 | 21.800 | 35.454 | 46.787 | 1.00 40.29 | SOLV |
| HETATM | 3211 | | TAW | 225 | 15.751 | 40.989 | 66.295 | 1.00 32.73 | SOLV |
| HETATM | 3212 | | WAT | 226 | 23.844 | 48.662 | 55.117 | 1.00 49.99 | SOLV |
| HETATM | 3213 | | TAW: | | 47.225 | 20.562 | 50.565 | 1.00 49.99 | SOLV |
| HETATM | 3214 | OH2 | TAW | 228 | 23.426 | 19.272 | 30.363 | 1.00 30.07 | 5524 |
| | | | | | | | | | |

| | | | | | 1. | iguic 17-1 | l . | | | | | |
|--------|----------|----------|-----|----|----------------|------------|------------------|--------|------|-------|-------|-------|
| | | | | | Residue | # X | Y | Z | occ. | В | Segme | nt ID |
| ATOM | 1 | СВ | ALA | A | 2 | 43.739 | 36.862 | 75.052 | 1.00 | 64.01 | 6 | |
| ATOM | 2 | c | ALA | | 2 | 44.405 | 38.106 | 72.971 | 1.00 | 60.02 | 6 | |
| ATOM | 3 | ō | ALA | | 2 | 43.251 | 38.536 | 72.908 | 1.00 | 57.94 | 8 | |
| | 4 | N | ALA | | 2 | 46.142 | 37.179 | 74.497 | | 62.88 | 7 | |
| ATOM | | CA | ALA | | 2 | 44.776 | 36.966 | 73.923 | | 63.02 | 6 | • |
| ATOM | 5 | | | | 3 | 45.398 | 38.588 | 72.233 | | 55.40 | 7 | |
| ATOM | 6 | N | LYS | | | | 39.671 | 71.287 | | 53.02 | 6 | |
| ATOM | 7 | CA | LYS | | 3 | 45.196 | | 70.421 | | 53.02 | 6 | |
| ATOM | 8 | CB | LYS | | 3 | 46.443 | 39.830 | | | 57.36 | 6 | |
| ATOM | 9 | CG | LYS | | | 47.703 | 40.093 | 71.217 | | 60.94 | 6 | |
| MOTA | 10 | CD | LYS | | 3 | 48.941 | 39.976 | 70.349 | | 63.48 | 6 | |
| ATOM | 11 | CE | LYS | | 3 | 48.909 | 40.957 | 69.196 | | | 7 | |
| ATOM | 12 | NZ | LYS | | 3 | 50.075 | 40.765 | 68.294 | | 66.87 | | |
| MOTA | 13 | С | LYS | | 3 | 43.986 | 39.401 | 70.399 | | 50.49 | 6 | |
| MOTA | 14 | 0 | LYS | | 3 | 43.691 | 38.255 | 70.063 | | 52.50 | 8 | |
| MOTA | 15 | N | VAL | | 4 | 43.281 | 40.464 | 70.034 | | 45.96 | 7 | |
| MOTA | 16 | CA | VAL | Α | 4 | 42.122 | 40.352 | 69.167 | | 41.16 | 6 | |
| ATOM | 17 | CB | VAL | | 4 | 40.983 | 41.272 | 69.638 | | 41.53 | 6 | |
| ATOM | 18 | CG1 | VAL | Α | 4 | 39.734 | 41.028 | 68.797 | | 40.07 | 6 | |
| MOTA | 19 | CG2 | VAL | A. | . 4 | 40.705 | 41.033 | 71.115 | | 38.31 | 6 | |
| MOTA | 20 | С | VAL | Ä | 4 | 42.519 | 40.796 | 67.796 | | 39.96 | 6 | |
| MOTA | 21 | 0 | VAL | Α | 4 | 43.123 | 41.914 | 67.645 | | 39.15 | 8 | |
| MOTA | 22 | N | LYS | A | 5 | 42.486 | 39.916 | 66.807 | | 36.24 | 7 | |
| MOTA | 23 | CA | LYS | A | 5 | 42.956 | 40.186 | 65.449 | | 35.66 | 6 | |
| ATOM | 24 | CB | LYS | Α | 5 | 43.930 | 39.088 | 65.024 | | 37.33 | 6 | |
| ATOM | 25 | ĊG | LYS | | 5 | 45.197 | 38.978 | 65.860 | 1.00 | 38.24 | 6 | • |
| ATOM | 26 | CD | LYS | | ['] 5 | 46.113 | 40.179 | 65.659 | 1.00 | 35.41 | 6 | |
| ATOM | 27 | CE | LYS | | 5 | 47.436 | 39.957 | 66.369 | 1.00 | 37.46 | 6 | |
| ATOM | 28 | NZ | LYS | | 5 | 48.345 | 41.121 | 66.245 | 1.00 | 35.63 | 7 | |
| ATOM | 29 | C | LYS | | 5 | 41.840 | 40.254 | 64.415 | 1.00 | 34.40 | 6 | |
| ATOM | 30 | ŏ | LYS | | 5 | 40.788 | 39.641 | 64.588 | 1.00 | 33.92 | 8 | |
| ATOM | 31 | N | LEU | | 6 | 42.082 | 40.983 | 63.329 | 1.00 | 32.52 | 7 | |
| ATOM | 32 | CA | LEU | | 6 | 41.097 | 41.094 | 62.253 | 1.00 | 33.64 | 6 | |
| ATOM | 33 | СВ | LEU | | 6 | 40.589 | 42.532 | 62.114 | 1.00 | 31.83 | 6 | |
| ATOM | 34 | CG | LEU | | 6 | 39.346 | 42.823 | 61.248 | 1.00 | 32.93 | 6 | |
| ATOM | 35 | | LEU | | 6 | 39.356 | 44.295 | 60.899 | 1.00 | 28.95 | 6 | |
| ATOM | 36 | | LEU | | 6 | 39.336 | 42.031 | 59.964 | | 32.87 | 6 | |
| | 37 | C | LEU | | 6 | 41.802 | 40.721 | 60.955 | | 35.09 | 6 | |
| MOTA | 38 | Ö | LEU | | 6 | 42.631 | 41.491 | 60.468 | | 36.93 | 8 | |
| MOTA | 39 | N | ILE | | 7 | 41.494 | 39.561 | 60.382 | | 35.52 | 7 | |
| ATOM | 40 | CA | ILE | | | 42.145 | 39.199 | 59.129 | | 35.14 | 6 | |
| ATOM | 41 | CB | ILE | | 7 | 42.062 | 37.711 | 58.850 | | 33.68 | 6 | |
| ATOM | 42 | | ILE | | 7 | 42.731 | 37.409 | 57.517 | 1.00 | 32.87 | 6 | |
| ATOM | 43 | | ILE | | 7 | 42.746 | 36.941 | 59.975 | | 33.32 | 6 | |
| ATOM | 44 | | ILE | | 7 . | 42.744 | 35.451 | 59.755 | | 35.09 | 6 | |
| MOTA | 45 | | ILE | | | 41.487 | | | | 37.13 | 6 | |
| MOTA | | | ILE | | 7 | 40.258 | 39.933 | 57.855 | | 35.21 | 8 | |
| MOTA | 46 47 | N | GLY | | 8 | 42.304 | 40.563 | 57.124 | | 37.25 | 7 | |
| MOTA | | CA | GLY | | 8 | 41.771 | 41.305 | 55.994 | | 38.69 | 6 | |
| ATOM 1 | 48 | | | | | 42.809 | 41.939 | 55.079 | | 39.73 | 6 | |
| ATOM | 49 | C | GLY | | 8 | 44.015 | 41.827 | 55.321 | | 39.21 | 8 | |
| ATOM | 50 | 0 | GLY | | 8 | | | 54.033 | | 39.41 | 7 | |
| MOTA | 51 | N | THR | | 9 | 42.335 | 42.622 43.268 | 53.057 | | 38.69 | 6 | |
| ATOM | 52 | CA | THR | | 9 | 43.212 | | 52.390 | | 37.27 | 6 | |
| MOTA | 53 | CB | THR | | 9 | 44.132 | 42.210 | 51.230 | | 36.82 | 8 | |
| ATOM | 54 | 0G1 | | | 9 | 44.754 | 42.771 | | | 38.59 | | |
| ATOM | 55 | | THR | | 9 | 43.332 | 40.972 | 52.001 | | | _ | |
| ATOM | 56 | С | THR | | 9 | 42.447 | 44.045 | 51.970 | | 38.60 | | |
| ATCM | 57 | 0 | THR | | 9 | 41.434 | 43.569 | 51.452 | | 37.30 | | |
| MOTA | 58 | N | LEU | | 10 | 42.939 | 45.238 | 51.628 | | 38.14 | | |
| MOTA | 59 | CA | LEU | Α | 10 | 42.304 | 46.077 | 50.609 | | 39.39 | | |
| ATOM | 60 | CB | LEU | A | 10 | 43.026 | 47.418 | 50.456 | | 38.98 | | |
| ATOM | €1 | CG | LEU | | 10 | 42.836 | 48.506 | 51.510 | | 39.68 | | |
| ATOM | 62 | | LEU | | 10 | 41.343 | 48.830 | 51.594 | | 40.22 | | |
| ATOM | 63 | | LEU | | 10 | 43.382 | 48.057 | 52.857 | | 40.11 | | |
| ATOM | 64 | c | LEU | | 10 | 42.238 | 45.432 | 49.239 | | 41.66 | | |
| 'ATOM | 65 | Ö | LEU | | 10 | 41.462 | 45.863 | 48.381 | | 42.08 | | |
| ATOM | 55 | N | ASP | | 11 | 43.052 | 44.408 | 49.025 | 1.00 | 43.51 | 7 | • |
| A+ C11 | | • • | | | | – | | _ | | | | |

| | 67 CA ASP A 11 | 43.071 | 43.731 4 | | 1.00 47.27 | 6 |
|--------------|------------------------------------|------------------|----------------------|------------------|--------------------------|--------|
| ATOM | 0, 011 1155 | 44.250 | | | 1.00 51.03 | 6 |
| ATOM | 68 CB ASP A 11 69 CG ASP A 11 | 45.579 | | | 1.00 54.10 | 6 8 |
| ATOM | 70 OD1 ASP A 11 | 45.944 | | | 1.00 55.93 | 8 |
| ATOM | 71 OD2 ASP A 11 | 46.255 | | | 1.00 57.79 1.00 46.36 | 5 |
| ATOM | 72 C ASP A 11 | 41.756 | | | 1.00 43.49 | 8 |
| ATOM | 73 O ASP A 11 | 41.472 | | | 1.00 46.80 | 7 |
| ATOM ATOM | 74 N TYR A 12 | 40.954 | | | 1.00 45.92 | 6 |
| ATOM | 75 CA TYR A 12 | 39.654 | | | 1.00 43.32 | 6 |
| ATOM | 76 CB TYR A 12 | 38.953 | | 49.030 50.390 | 1.00 38.82 | 6 |
| ATOM | 77 CG TYR A 12 | 39.358 | | 51.775 | 1.00 37.95 | 6 |
| ATOM | 78 CD1 TYR A 12 | 39.531 | 40.720 39.560 | 52.476 | 1.00 36.18 | 6 |
| ATOM | 79 CE1 TYR A 12 | 39.869 | 39.300 | 49.721 | 1.00 37.69 | 6 |
| ATOM | 80 CD2 TYR A 12 | 39.533 | 38.316 | 50.415 | 1.00 35.83 | 6 |
| ATOM | 81 CE2 TYR A 12 | 39.868 40.032 | 38.365 | 51.787- | 1.00 34.10 | 6 |
| MOTA | 82 CZ TYR A 12 | 40.339 | 37.216 | 52.470 | 1.00 36.31 | 8 |
| ATOM | 83 OH TYR A 12 84 C TYR A 12 | 38.786 | 42.966 | 47.378 | 1.00 46.56 | 6 |
| MOTA | | 37.821 | 42.476 | 46.791 | 1.00 47.38 | 8 |
| ATOM | 13 | 39.138 | 44.247 | 47.278 | 1.00 47.28 | 7 |
| ATOM | 86 N GLY A 13 87 CA GLY A 13 | 38.385 | 45.164 | 46.442 | 1.00 46.53 | 6 |
| ATOM | 88 C GLY A 13 | 38.650 | 44.934 | 44.968 | 1.00 45.60 1.00 43.68 | 8 |
| ATOM | 89 O GLY A 13 | 37.895 | 45.401 | 44.117 | 1.00 46.52 | 7 |
| MOTA MOTA | 90 N LYS A 14 | 39.725 | 44.210 | 44.672 43.296 | 1.00 47.28 | 6 |
| MOTA | 91 CA LYS A 14 | 40.112 | 43.908 | 43.290 | 1.00 50.22 | 6 |
| ATOM | 92 CB LYS A 14 | 41.629 | 43.748 45.044 | 43.307 | 1.00 57.12 | 6 |
| ATOM | 93 CG LYS A 14 | 42.396 42.038 | 46.004 | 42.161 | 1.00 63.60 | 6 |
| MOTA | 94 CD LYS A 14 | 42.349 | 45.422 | 40.768 | 1.00 66.65 | 6 |
| MOTA | 95 CE LYS A 14 | 41.529 | 44.220 | 40.387 | 1.00 67.70 | 7 |
| ATOM - | JU 110 | 39.460 | 42.643 | 42.769 | 1.00 44.18 | 6 |
| MOTA | 97 C LYS A 14 98 O LYS A 14 | 39.564 | 42.325 | 41.585 | 1.00 40.33 | 8 7 |
| MOTA | 99 N TYR A 15 | 38.790 | 41.926 | 43.661 | 1.00 43.25 1.00 43.18 | 6 |
| MOTA MOTA | 100 CA TYR A 15 | 38.145 | 40.665 | 43.317 44.142 | 1.00 36.88 | 6 |
| MOTA | 101 CB TYR A 15 | 38.789 | 39.547 | 44.142 | 1.00 32.96 | 6 |
| MOTA | 102 CG TYR A 15 | 40.302 | 39.560 39.107 | 45.108 | 1.00 30.90 | 6 |
| ATOM | 103 CD1 TYR A 15 | 41.084 | 39.107 | 45.035 | 1.00 30.94 | 6 |
| ATOM | 104 CE1 TYR A 15 | 42.476 40.952 | 40.049 | 42.912 | 1.00 33.01 | 6 |
| MOTA | 105 CD2 TYR A 15 | 42.341 | 40.092 | 42.826 | 1.00 29.68 | 6 |
| MOTA | 106 CE2 TYR A 15 | 43.098 | | 43.890 | 1.00 30.99 | 6 |
| atom | 10, 00 110 | 44.471 | 39.673 | 43.809 | 1.00 28.02 | 8 |
| ATOM | 108 OH TYR A 15 109 C TYR A 15 | 36.661 | | 43.621 | 1.00 45.56 | 6 8 |
| MOTA | 110. O TYR A 15 | 36.149 | 40.153 | 44.552 | 1.00 45.22 1.00 48.81 | 7 |
| ATOM ATOM | 111 N ARG A 16 | 35.981 | | 42.830 42.999 | 1.00 53.22 | 6 |
| ATOM | 112 CA ARG A 16 | 34.553 | 41.819 | 42.554 | 1 0 57.11 | 6 |
| ATOM | 113 CB ARG A 16 | 34.193 | | 43.490 | | 6 |
| ATOM | 114 CG ARG A 16 | 34.852 34.280 | | 44.886 | 1.00 67.04 | 6 |
| MOTA | 115 CD ARG A 16 | 34.798 | | 45.569 | 1.00 73.59 | 7 |
| ATOM | 116 NE ARG A 16 | 34.612 | | 45.141 | 1.00 75.03 | 6 |
| ATOM | | 33.91 | | 44.033 | | 7 7 |
| ATOM | 120 | 35.142 | 47.856 | 45.808 | | 6 |
| ATOM | 119 NH2 ARG A 16 120 C ARG A 16 | 33.75 | 7 40.903 | | | 8 |
| ATOM | 121 O ARG A 16 | 34.19 | | | 1.00 50.89 | . 7 |
| MOTA | 122 N TYR A 17 | 32.59 | 5 40.463 | 42.552 | | 6 |
| MOTA. | 123 CA TYR A 17 | 31.73 | 7 39.634 | 41.733 | | 6 |
| atom atom | 124 CB TYR A 17 | 30.53 | 4 39.119 | | | 6 |
| ATOM | 125 CG TYR A 17 | 30.80 | 3 37.894 9 37.932 | | | 6 |
| ATOM | 126 CD1 TYR A 17 | 31.58 | | | 1.00 43.36 | 6 |
| ATOM | 127 CE1 TYR A 17 | 31.96 30.18 | | | 1.00 39.89 | 6 |
| ATOM | 128 CD2 TYR A 17 | 30.44 | | | 1.00 40.56 | 6 |
| ATCM | 129 CE2 TYR A 17 | 31.33 | | | 9 1.00 41.98 | 6 |
| ATOM | 130 CZ TYR A 17 | 31.60 | 0 34.438 | 3 45.59 | | |
| ATOM | | 31.24 | | 7 40.62 | 2 1.00 51.88 | , 0 |
| ATOM. | 132 C TYR A 1/ | • | | • | | |
| - | | | | | | |

Figure 17-3

| . =0.1 | 133 0 | TYR A | 17 | 31.332 | 41.772 | | 1.00 47.86 | 8 7 |
|--------------|----------------|--------------------|----------|------------------|------------------|------------------|--------------------------|----------|
| ATOM | 134 N | PRO A | 18 | 30.730 | 39.964 | | 1.00 54.38 1.00 54.21 | 6 |
| ATOM ATOM | 135 CD | PRO A | 18 | 30.548 | 38.545 | 39.190 | 1.00 54.21 | 6 |
| ATOM | 136 CA | PRO A | 18 | 30.243 | 40.809 | 38.449 37.496 | 1.00 56.84 | 6 |
| ATOM | 137 CB | | 18 | 29.601 | 39.792 | 38.426 | 1.00 56.46 | 6 |
| ATOM - | 138 CG | PRO A | 18 | 29.260 | 38.613 | 38.932 | 1.00 58.74 | 6 |
| ATOM | 139 C | PRO A | 18 | 29.273 | 41.891 41.861 | 40.066 | 1.00 55.72 | 8 |
| ATOM | 140 0 | PRO A | 18 | 28.791 | 41.861 | 38.052 | 1.00 62.10 | 7 |
| AŢOM | 141 N | LYS A | 19 | 29.017 28.127 | 42.631 | 38.314 | 1.00 64.85 | 6 |
| ATOM | 142 CA | | 19 | 27.972 | 44.781 | 37.022 | 1.00 69.74 | 6 |
| MOTA | 143 CB | | 19 19 | 28.008 | 43.925 | 35.740 | 1.00 74.99 | 6 |
| MOTA | 144 CG | | 19 . | 26.895 | 42.881 | 35.668- | 1.00 78.18 | 6 |
| MOTA | 145 CE | _ | 19 | 26.981 | 42.010 | 34.420 | 1.00 80.24 | 6 |
| MOTA | 146 CE | | 19 | 25.867 | 41.010 | 34.361 | 1.00 81.13 | 7 |
| MOTA | 148 C | LYS A | 19 | 26.750 | 43.619 | 38.869 | 1.00 64.77 1.00 66.50 | 6 - 8 |
| ATOM ATOM | 149 0 | LYS A | 19 | 26.414 | 43.961 | 40.001 38.062 | 1.00 63.75 | 7 |
| ATOM | 150 N | ASN A | 20 | 25.957 | 42.933 | 38.439 | 1.00 62.96 | 6 |
| MOTA | 151 CA | | 20 | 24.612 | 42.556 42.031 | 37.208 | 1.00 67.42 | 6 |
| ATOM | 152 CI | | 20 | 23.870 22.392 | 42.031 | 37.459 | 1.00 72.29 | 6 |
| MOTA | 153 CC | | 20 | 22.392 | 42.785 | 37.772 | 1.00 75.25 | 8 |
| MOTA | | O1 ASN A | 20 | 21.000 | 40.594 | 37.322 | 1.00 74.38 | 7 |
| ATOM | | D2 ASN A | 20 20 | 24.602 | 41.512 | 39.547 | 1.00 61.30 | 6 |
| MOTA | 156 C | ASN A ASN A | 20 | 23.629 | 40.773 | 39.698 | 1.00 61.49 | 8 |
| ATOM | 157 O 158 N | | 21 | 25.681 | 41.444 | 40.321 | 1.00 57.30 | 7 6 |
| MOTA | 159 C | | 21 | 25.755 | 40.480 | 41.418 | 1.00 54.68 1.00 52.63 | 6 |
| MOTA MOTA | 160 C | | 21 | 27.071 | 39.700 | 41.373 | 1.00 49.39 | 6 |
| MOTA | 161 C | | .21 | 27.058 | 38.449 | 42.195 43.503 | 1.00 49.39 | 6 |
| MOTA | | D2 HIS A | 21 | 27.336 | 38.236 37.229 | 41.686 | 1.00 48.27 | 7 |
| ATOM | | D1 HIS A | 21 | 26.664 26.704 | 36.320 | 42.643 | 1.00 48.16 | 6 |
| MOTA | | E1 HIS A | 21 | 27.108 | 36.905. | 43.757 | 1.00 47.33 | 7 |
| MOTA | | E2 HIS A | 21 21 | 25.664 | 41.215 | 42.760 | 1.00 52.89 | 6 |
| ATOM | 166 C | | 21 | 26.295 | 42.256 | 42.947 | 1.00 52.52 | 8 7 |
| MOTA | 167 O | | 22 | 24.880 | 40.679 | 43.713 | 1.00 50.81 | 6 |
| MOTA MOTA | | D PRO A | 22 | 24.076 | 39.444 | 43.661 | 1.00 48.50 1.00 48.02 | 6 |
| ATOM | | A PRO A | 22 | 24.734 | 41.310 | 45.029 45.783 | 1.00 47.45 | 6 |
| ATOM | | B PRO A | 22 | 23.860 | 40.308 39.754 | 44.667 | 1.00 47.76 | 6 |
| ATOM | 172 C | G PRO A | 22 | 22.990 26.074 | | 45.727 | 1.00 46.48 | 6 |
| ATOM | 173 C | | 22 | 26.164 | | 46.615 | 1.00 45.69 | 8 |
| ATOM | 174 0 | | 22 23 | 27,107 | | | 1.00 44.97 | 7 |
| ATOM | 175 N | | | 28.441 | 40.949 | | 1.00 41.31 | 6 |
| ATOM | | A LEU A B LEU A | | 29.076 | 39.569 | | 1.00 39.22 | 6 6 |
| ATOM ATOM | | G LEU A | | 28.264 | | | 1.00 37.71 1.00 35.07 | 6 |
| ATOM | 179 | Di LEU A | 23 | 29.075 | | | | 6 |
| ATOM | 180 | DL LEU A | . 23 | 27.896 | 39.165 | | | 6 |
| ATOM | 181 (| LEU A | | 29.334 | | | | 8 |
| ATOM | | LEU A | | 30.556 28.706 | | | 1.00 39.67 | 7 |
| ATOM | | N LYS A | | 29.430 | | 43.398 | 1.00 42.88 | 6 |
| ATOM | | CA LYS A | | 28.480 | | | 1.00 40.24 | 6 |
| MOTA | | CB LYS A | | 28.94 | | 41.610 | | 6 |
| MOTA | | CG LYS A | | 28.24 | | 42.166 | | 6 6 |
| MOTA | | CE LYS ? | | 26.73 | 2 46.492 | | | 7 |
| ATOM | | NZ LYS ? | | 25.98 | 9 47.71 | 7 42.362 | | |
| MOTA ATOM | | C LYS A | | 30.03 | 1 44.72 | | | |
| ATOM | | O LYS F | 24 | 31.02 | | | | |
| ATOM | | N ILE ? | A 25 | 29.43 | | - | | 6 |
| ATOM | 193 | CA ILE A | | 29.87 | | | 1.00 37.72 | . 6 |
| atom | | CB ILE | | 28.76 27.53 | | | 1.00 39.67 | 6 |
| ATOM | 195 | CG2 ILE | | 28.41 | | 8 48.14 | 5 1.00 35.25 | |
| ATOM | | CG1 ILE | _ | 27.30 | 1 45.36 | 8 49.15 | | |
| ATOM | | CD1 ILE 2 | ·- | 31.07 | | 5 47.11 | 2 1.00 40.23 | 6 |
| ATCM | 198 | C ILE | | | | - | | |

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| | | | | | | | | 44 444 | 47.198 | 1.00 38.90 | 8 |
|------|-----|------|-------|-----|------|-----|--------|---------|------------------|---------------|-----|
| MOTA | 199 | 0 | ILE | À | 25 | 31 | .419 | 44.441 | - | | 7 |
| | | | PRO | | 26 | 31 | .762 | 46.616 | 47.709 | 1.00 40.18 | |
| MOTA | 200 | N | | | | | .523 | 48.051 | 47.533 | 1.00 40.58 | 6 |
| ATOM | 201 | ÇD | PRO | À | 26 | | | | | 1.00 38.31 | 6 |
| | 202 | CA | PRO | A | 26 | 32 | .939 | 46.437 | 48.558 | | |
| atom | | | | | 26 | | .478 | 47.860 | 48.688 | 1.00 37.14 | 6 |
| ATOM | 203 | CB | PRO | | | | | 48.537 | 47.458 | 1.00 38.77 | 6 |
| ATOM | 204 | CG | PRO | A | 26 | | .940 | | 47.450 | 1 00 37 33 | 6 |
| - | 205 | c | PRO | Δ | 26 | 32 | . 433 | 45.903 | 49.891 | 1.00 37.32 | |
| MOTA | | | | | | 2.1 | .416 | 46.372 | 50.412 | 1.00 32.70 | 8 |
| MOTA | 206 | 0 | PRO | Ä | 26 | | | | 50.452 | 1.00 36.54 | 7 |
| | 207 | N | ARG | A | 27 | 33 | .134 | 44.930 | 50.452 | | 6 |
| ATOM | | | ARG | | 27 | 32 | .685 | 44.359 | 51.711 | 1.00 37.39 | |
| ATCM | 208 | CA | | | | | .116 | 42.952 | 51.455 | 1.00 35.29 | 6 |
| MOTA | 209 | CB | ARG | A | 27 | | | | 50.355 | 1.00 32.69 | 6 |
| ATOM | 210 | CG | ARG | À | 27 | 31 | .047 | 42.956 | 50.333 | 1.00 32.03 | 6 |
| | | | ARG | | 27 | 30 | .507 | 41.573 | 49.956 | 1.00 33.87 | |
| MOTA | 211 | CD | | | | | .757 | 40.909 | 51.021 | 1.00 36.16 | 7 |
| ATOM | 212 | NE | ARG | A | 27 | | | 40.202 | 51.959 | 1.00 37.11 | 6 |
| ATOM | 213 | CZ | ARG | À | 27 | | .293 | 40.132 | 31.333 | | 7 |
| | | | ARG | | 27 | 31 | .604 | 39.903 | 51.976 | 1.00 34.42 | |
| ATOM | 214 | | | | | | .516 | 39.597 | 52.896 | 1.00 33.67 | 7 |
| ATOM | 215 | NH2 | ARG | | 27 | | | 44.329 | 52.732 | 1.00 36.35 | 6 |
| ATOM | 216 | С | ARG | Ä | 27 | _ | .813 | | | 1.00 35.77 | 8 |
| | 217 | ō | ARG | | 27 | 33 | .881 | 45.188 | 53.610 | | |
| ATOM | | | | | | | .703 | 43.351 | 52.607 | 1.00 34.93 | 7 |
| MOTA | 218 | N | VAL | | 28 | | | 43.230 | 53.537 | 1.00 34.00 | 6 |
| ATOM | 219 | CA | VAL | Α | 28 | | .810 | | 55.557 | | 6 |
| | 220 | СВ | VAL | 2 | 28 | 36 | .633 | 41.954 | 53.252 | | |
| MOTA | | | | | | 37 | .574 | 41.652 | 54.424 | 1.00 33.59 | 6 |
| ATOM | 221 | | VAL | | 28 | | | 40.790 | 52.992 | 1.00 37.05 | 6 |
| ATOM | 222 | CG2 | VAL | A | 28 | | . 696 | | | 1.00 31.91 | 6 |
| | 223 | C | VAL | | 28 | 36 | .712 | 44.454 | 53.423 | | |
| ATOM | | | | | 28 | 37 | .216 | 44.959 | 54.427 | 1.00 31.45 | 8 |
| ATOM | 224 | 0 | VAL | | | | | 44.936 | | 1.00 33.12 | 7 |
| MOTA | 225 | N | SER | Α | 29 | | .908 | | - | 1.00 32.03 | 6 |
| | 226 | CA | SER | A | 29 | 37 | 7.751 | 46.111 | | | |
| MOTA | | | | | 29 | 3.5 | 3.205 | 46.181 | 50.499 | 1.00 31.77 | 6 |
| MOTA | 227 | CB | SER | | | | 7.113 | 46.223 | 49.600 | 1.00 30.80 | 8 |
| ATOM | 228 | OG . | SER | A | 29 | _ | | | | | 6 |
| | 229 | С | SER | A | 29 | 37 | 7.003 | 47.380 | | | 8 |
| MOTA | | | | | 29 | 3. | 7.604 | 48.404 | 52.650 | | |
| MOTA | 230 | 0 | SER | | | | 5.682 | 47.310 | 52.352 | 1.00 32.43 | 7 |
| MOTA | 231 | N | LEU | Α | 30 | | | | | - - | 6 |
| MOTA | 232 | CA | LEU | Α | 30 | 34 | 4.900 | 48:465 | | | 6 |
| | | | LEU | | 30 | 3: | 3.463 | 48.358 | 52.221 | | |
| MOTA | 233 | CB | | | | | 2.508 | 49.513 | 52.560 | 1.00 36.79 | 6 |
| MOTA | 234 | CG | LEU | | 30 | | | 49.446 | | | 6 |
| ATOM | 235 | CD1 | LEU | À | 30 | | 2.070 | | | | 6 |
| | 236 | CD2 | | | 30 | 3. | 3.202 | 50.840 | 52.256 | | |
| MOTA | | | | | | | 4.902 | 48.527 | 54.262 | 1.00 34.89 | 6 |
| ATOM | 237 | С | LEU | | 30 | | | 49.601 | | 1.00 37.58 | 8 |
| MOTA | 238 | 0 | LEU | A | 30 | | 5.033 | | | | 7 |
| | 239 | N | LEU | 4 1 | 31 | 3 | 4.761 | 47.366 | 5 54.897 | | |
| ATOM | | | | | 31 | ٦ | 4.743 | 47.276 | 56.350 | 1.00 34.85 | 6 |
| ATOM | 240 | CA | LEU | | | | | 45.808 | | 1.00 36.37 | 6 |
| ATCM | 241 | CB | LEU | J A | 31 | | 4.768 | | | | 6 |
| | 242 | CG | LEU | I A | 31 | 3 | 4.459 | 45.47 | | | 6 |
| MOTA | | | LEU | | 31 | 3 | 4.841 | 44.02 | 7 58.532 | | |
| ATOM | 243 | ردی | LLEU | _ ^ | | | 5.228 | 46.35 | | 1.00 35.86 | . 6 |
| ATOM | 244 | CD2 | LEU | J A | 31 | | | | | | . 6 |
| MOTA | 245 | С | LEU | JÀ | 31 | 3 | 5.976 | 47.99 | | | 8 |
| | 246 | ō | LEU | | 31 | 3 | 5.855 | 49.03 | | | |
| atom | | | | | | 2 | 7.157 | 47.42 | 6 56.63 | 5 1.00 37.76 | 7 |
| ATOM | 247 | N | LEU | | 32 | | | | | | 6 |
| ATCM | 248 | CA | LEU | JA | 32 | | 8.420 | | | | 6 |
| | 249 | CB | LEU | | 32 | 3 | 9.611 | 47.31 | | | |
| atom | | | | | | | 0.030 | | 8 56. <i>774</i> | 4 1.00 39.11 | 6 |
| ATOM | 250 | CG | LE | | 32 | | | | | | 6 |
| ATOM | 251 | CD: | i LEU | JΑ | 32 | | 1.117 | | | | 6 |
| | 252 | | 2 LEC | | | 4 | 0.538 | 45.83 | | | |
| ATOM | | | | | | | 8.500 | | 3 56.78 | 0 1.00 34.84 | 6 |
| ATOM | 253 | С | | Αţ | | | | | | | . 8 |
| ATOM | 254 | 0 | LE | JA | 32 | | 8.846 | | | | |
| | | N | | 3 A | | 3 | 8.184 | | | | |
| ATOM | 255 | | | | | | 8.247 | | 0 55.15 | | 6 |
| ATOM | 256 | CA | | 3 A | | | | | | | 6 |
| ATOM | 257 | CB | AR | G A | . 33 | | 7.927 | | | | |
| | | | | G A | _ | 7 | 8.481 | 52.65 | | | |
| atom | 258 | CG | | | | | 8.107 | | | 1 1.00 43.44 | 6 |
| ATCM | 259 | CD | | G A | | | | | | | 7 |
| ATCM | 260 | | AR | G À | 33 | | 8.521 | | | | |
| | | | | GΑ | | - 1 | 38.348 | 3 51.46 | 9 49.49 | | |
| atom | 261 | | | | | | 37.771 | | 9 48.82 | 3 1.00 51.75 | |
| ATCM | 262 | | 1 AR | | | | | | 9 48.85 | | 3 7 |
| ATCM | 263 | NH | 2 AR | G A | 33 | | 38.739 | | | | |
| | | | | G A | | : | 37.274 | 52.10 | 02 _55.98 | 5 4.00 Jan.J. | • |
| atom | 264 | _ | - AN | | | | | | - | | |

| | | | | | • | | | | | |
|--------|------|-----|-------|-------|---|--------|----------|----------------|------------|-----|
| | 265 | ^ | ARG A | 33 | | 37.471 | 53.299 | 56.196 | 1.00 29.23 | 8 |
| MOTA | 265 | ~ | | 34 | | 36.231 | 51.445 | 56.484 | 1.00 32.58 | 7 |
| MOTA | 266 | N | PHE A | 34 | | 35.216 | 52.096 | 57.304 | 1.00 32.69 | 6 |
| ATOM | 267 | CA | PHE A | | | 33.952 | 51.232 | 57.359 | 1.00 31.22 | 6 |
| MOTA | 268 | CB | PHE A | 34 | | 32.838 | 51.825 | 58.183 | 1.00 28.74 | 6 |
| ATOM | 269 | CG | PHE A | 34 | | | 52.888 | 57.700 | 1.00 22.76 | 6 |
| ATOM | 270 | CD1 | PHE A | 34 | | 32.085 | | 59.456 | 1.00 28.09 | 6 |
| ATOM | 271 | CD2 | PHE A | 34 | | 32.551 | 51.322 | 59.450 | 1.00 23.70 | 6 |
| ATOM | 272 | CE1 | PHE A | 34 | | 31.061 | 53.441 | 58.472 | 1.00 23.70 | 6 |
| | 273 | CE2 | PHE A | 34 | | 31.524 | 51.873 | 60.235 | 1.00 24.59 | |
| ATOM | 274 | CZ | PHE A | 34 | | 30.781 | 52.929 | 59.741 | 1.00 21.39 | 6 |
| ATOM | 275 | C | PHE A | | | 35.734 | 52.319 | 58.719 | 1.00 33.45 | 6 |
| MOTA | | | PHE A | | | 35.635 | 53.425 | 59.258 | 1.00 35.49 | 8 |
| MOTA | 276 | 0 | LYS A | _ | | 36.276 | 51.264 | 59.323 | 1.00 34.52 | 7 |
| MOTA | 277 | N | | | | 36.805 | 51.360 | 60.678 | 1.00 36.51 | 6 |
| MOTA | 278 | CA | LYS A | | | 37.118 | 49.977 | 61.235 | 1.00 36.47 | 6 |
| MOTA | 279 | CB | LYS A | | | 35.912 | 49.074 | 61.343 | 1.00 40.81 | 6 |
| MOTA | 280 | CG | LYS A | | | 36.246 | 47.801 | 62.090 | 1.00 44.10 | 6 |
| ATOM | 281 | CD | LYS A | | | 37.347 | 47.029 | 61.402 | 1.00 47.46 | 6 |
| ATOM | 282 | CE | LYS A | | | | 47.823 | 61.276 | 1.00 53.53 | 7 |
| MOTA | 283 | NZ | LYS A | | | 38.601 | 52.222 | 60.735 | 1.00 36.61 | 6 |
| MOTA | 284 | С | LYS A | | | 38.054 | 52.824 | 61.766 | 1.00 36.78 | 8 |
| MOTA | 285 | 0 | LYS A | . 35 | | 38.352 | 52.624 | 59.635 | 1.00 36.27 | 7 |
| ATOM | 286 | N | ASP A | 36 | | 38.794 | 52.267 | | 1.00 39.71 | 6 |
| MOTA | 287 | CA | ASP A | 36 | | 39.980 | 53.090 | 59.592 | 1.00 44.78 | 6 |
| ATOM | 288 | CB | ASP A | 36 | | 40.679 | 52.937 | 58.239 | | 6 |
| ATOM | 289 | CG | ASP A | 36 | | 41.863 | 53.892 | 58.075 | | 8 |
| MOTA | 290 | | ASP A | 36 | | 42.803 | 53.352 | 58.906 | 1.00 44.02 | 8 |
| ATOM | 291 | | ASP A | | | 41.843 | 54.682 | 57.106 | 1.00 48.43 | 6 |
| - | 292 | c | ASP A | | | 39.508 | 54.530 | 59.789 | 1.00 39.99 | |
| ATOM - | 293 | ō | ASP A | | | 40.023 | 55.258 | 60.536 | 1.00 40.76 | 8 |
| ATOM | 294 | N | ALA A | _ | | 38.506 | 54.919 | 59.00 7 | 1.00 38.59 | 7 |
| MOTA | | CA | ALA A | | | 37.939 | 56.258 | 59.066 | 1.00 37.14 | 6 |
| ATOM | 295 | | ALA A | | | 36.857 | 56.402 | 58.000 | 1.00 35.85 | 6 |
| MOTA | 296 | CB | | | | 37.354 | 56.549 | 60.446 | 1.00 38.34 | 6 |
| MOTA | 297 | C | ALA A | - : - | | 37.391 | 57.687 | 60.928 | 1.00 37.32 | 8 |
| MOTA | 298 | 0 | ALA A | - | | 36.809 | 55.518 | 61.079 | 1.00 36.19 | 7 |
| MOTA | 299 | N | MET A | | | 36.213 | 55.674 | 62.397 | 1.00 36.80 | 6 |
| MOTA | 300 | CA | MET A | _ | | 35.141 | 54.598 | 62.606 | 1.00 37.38 | 6 |
| ATOM | 301 | CB | MET A | | | 33.938 | 54.717 | 61.673 | 1.00 37.60 | 6 |
| ATOM | 302 | CG | MET A | | | 32.887 | 56.165 | 61.999 | 1.00 33.61 | 16 |
| MOTA | 303 | SD | MET | | | 32.398 | 55.824 | 63.680 | 1.00 35.60 | 6 |
| ATOM . | 304 | CE | MET A | | | 37.262 | 55.582 | 63.502 | 1.00 35.84 | 6 |
| MOTA | 305 | C | MET . | | | | 55.688 | 64.692 | 1.00 34.89 | 8 |
| ATOM | 306 | 0 | MET . | | | 36.937 | 55.400 | 63.100 | 1.00 33.83 | 7 |
| MOTA | 307 | N | ASN . | | | 38.518 | 55.264 | 64.044 | 1.00 34.94 | 6 |
| ATOM | 308 | CA | ASN . | | | 39.626 | | 64.775 | 1.00 32.48 | 6 |
| MOTA | 309 | CB | ASN . | | | 39.897 | 56.582 | 63.825 | 1.00 32.34 | 6 |
| ATOM | 310 | CG | ASN . | A 39 | | 40.213 | 57.717 | 63.009 | 1.00 31.85 | 8 |
| ATOM | 311 | OD: | ASN | A 39 | | 41.128 | 57.621 | | 1.00 30.92 | 7 |
| ATCM | 312 | ND2 | ASN . | A 39 | | 39.455 | 58.800 | 63.924 | 1.00 36.87 | 6 |
| MOTA | 313 | С | ASN | A 39 | | 39.253 | 54.183 | 65.045 | | 8 |
| ATOM | 314 | 0 | ASN | A 39 | | 39.403 | | 66.260 | | 7 |
| MOTA | 315 | N | LEU | | | 38.752 | | 64.518 | 1.00 37.48 | 6 |
| | 316 | CA | LEU | | | 38.341 | 51.933 | 65.336 | | 6 |
| ATOM | 317 | CB | LEU | _ | | 36.863 | 51.622 | 65.086 | | |
| ATOM | | CG | LEU | | | 35.858 | 52.712 | 65.476 | | 6 |
| ATOM | .318 | | 1 LEU | | | 34.448 | | 65.111 | | 6 |
| ATOM | 319 | | | | | 35.951 | | 66.966 | | 6 |
| MOTA | 320 | | 2 LEU | | | 39.184 | | | 1.00 39.79 | 6 |
| MOTA | 321 | C | LEU | | | 38.804 | | | 1.00 36.88 | 8 |
| MOTA | 322 | 0 | LEU | | | 40.337 | | | 1.00 40.50 | ? |
| ATOM | 323 | N | ILE | | | | | | | 6 |
| ATOM | 324 | CA | | | | 41.237 | | | | 6 |
| ATOM | 325 | | | | | 40.780 | | | | 6 |
| MOTA | 326 | CG | | | | 41.01 | | | | 6 |
| MOTA | 327 | | 1 ILE | A 41 | | 41.513 | | | | |
| ATOM | 328 | | 1 ILE | | | 41.08 | | | | . 6 |
| | 329 | | ILE | | | 42.68 | | | | 8 |
| ATOM | 330 | | ILE | | | 42.92 | 7 51,328 | 63.27 | 1.00 40.01 | • |

| | | | | | 4.7 | | 49.582 | 64.497 | 1.00 45 | .19 | 7 |
|--------------|------------|---------|--------|----------|-----|--------------|------------------|-----------------------|------------------|----------------|--------|
| ATOM | 331 N | | | 42 | | .646 .049 | 49.982 | 64.372 | 1.00 45 | . 62 | 6 |
| ATOM | 332 C | A A | - | 42 | | | 50.090 | 65.742 | 1.00 45 | 5.17 | 6 |
| MOTA | 333 CI | B A | SP A | 42 | 45 | .716 | 51.005 | 66.682 | 1.00 44 | | 6 |
| ATOM | 334 C | | SP A | 42 | | .966 | | 66.322 | | .84 | 8 |
| MOTA | 335 0 | D1 A | SP A | 42 | | .731 | 52.177 | 67.787 | 1.00 48 | | 8 |
| ATOM | 336 0 | D2 A | SP A | 42 | | .612 | 50.546 | 63.551 | 1.00 48 | | 6 |
| MOTA | 337 C | | SP A | 42 | | .750 | 48.915 | | | 9.85 | 8 |
| | 338 0 | | SP A | 42 | | .316 | 47.757 | 63.547 | 1.00 49 | | 7 |
| MOTA | 339 N | | LU A . | 43 | | .830 | 49.288 | 62.864 | | 0.79 | 6 |
| MOTA | | | LU A | 43 | 47 | 7.553 | 48.325 | 62.028 | | 9.90 | 6 |
| MOTA | | - | LU A | 43 . | 48 | 3.820 | 48.956 | 61.431 | | | 6 |
| MOTA | | | LUA | 43 | 4.8 | 3.544 | 50.029 | 60.378 | 1.00 5 | 7.20 9.56 | 6 |
| MOTA | • | - | LU A | 43 | 49 | 808. | 50.537 | 59.690 | | | 8 |
| ATOM | | | LU A | 43 | 50 |).517 | 49.721 | 59.061 | 1.00 6 | | 8 |
| MOTA | 345 0 | F2 G | LU A | 43 | 50 | 0.095 | 51.750 | 59.772 | | 7.82 | 6 |
| MOTA | 346 C | | LU A | 43 | 4 | 7.918 | 47.020 | 62.733 | 1.00 4 | | 8 |
| ATOM | 347 0 | | LU A | 43 | 4 | 7.813 | 45.943 | 62.149 | 1.00 4 | | 7 |
| ATOM | 348 N | _ | YS A | 44 | 4 | B.324 | 47.118 | 63.992 | | | 6 |
| MOTA | | | YS A | 44 | 4 | 8.730 | 45.949 | 64.762 | 1.00 4 | | 6 |
| MOTA | | | YS A | 44 | 4 | 9.317 | 46.418 | 66.093 | 1.00 5 1.00 5 | 2.46 | 6 |
| MOTA | | | YS A | 44 | 5 | 0.448 | 47.421 | 65.899 | 1.00 5 | 0.74 | 6 |
| MOTA | | | LYS A | 44 | | 1.167 | 47.749 | 67.201 | | 8.48 | 6 |
| ATOM | | | LYS A | 44 | 5 | 2.327 | 48.704 | 66.949 | | 8.95 | 7 |
| ATOM | | | LYS A | 44 | 5 | 3.122 | 48.968 | 68.176 | 1.00 5 | | 6 |
| MOTA | | | LYS A | 44 | 4 | 7.638 | 44.897 | 64.994 | | 15.13 | 8 |
| MOTA | _ | | LYS A | 44 | | 7.932 | 43.738 | 65.290 | 1.00 4 | | 7 |
| MOTA MOTA | | | GLU A | 45 | | 6.379 | 45.298 | 64.854 65.046 | 1.00 4 | 13.23. | 6 |
| ATOM | | CA (| GLU A | 45 | | 5.268 | 44.374 | 65.514 | | 11.19 | 6 |
| ATOM | | CB (| GLU A | 45 | 4 | 4.024 | 45,143 | 66.844 | | 36.83 | 6 |
| ATOM- | | CG (| GLU A | 45 | 4 | 4.192 | 45.859 46.741 | 67.204 | | 38.92 | 6 |
| MOTA | 361 | | GLU A | 45 | 4 | 3.003 | 47.701 | | 1.00 | | 8 |
| ATOM | 362 | | GLU A | 45 | | 2.707 | 46.479 | | | 36.33 | 8 |
| ATOM | 363 | | GLU A | 45 | | 4.969 | 43.660 | | 1.00 | 43.04 | 6 |
| MOTA | | _ | GLU A | 45 | | 4.480 | 42.523 | | | 45.03 | 8 |
| MOTA | • | | GLU A | 4.5 | | 5.282 | 44.341 | | | 40.29 | 7 |
| ATOM | • • • | | LEU A | 46 | | 5.042 | 43.823 | 61.299 | _ | 37.16 | 6 |
| MOTA | | | LEU A | 46 46 | | 4.910 | | 44 | | 37.86 | 6 |
| MOTA | | | LEU A | 46 | | 4.822 | | 58.845 | | 39.22 | 6 |
| MOTA | 369 | | LEU A | 46 | | 13.655 | | 58.563 | | 40.68 | 6 |
| ATOM | 370 | CDI | LEU A | 46 | | 44.673 | | 58.080 | | 41.62 | 6 6 |
| ATOM | 371 372 | | LEU A | 46 | | 46.090 | 42.860 | | | 36.54 | 8 |
| MOTA | 373 | 0 | LEU A | 46 | ٠, | 47.275 | 43.192 | 60.698 | | 39.86 33.49 | 7 |
| MOTA | 374 | N | ILE A | 47 | | 45.646 | | | | 30.51 | 6 |
| MOTA MOTA | 375 | CA | ILE A | 47 | | 46.540 | | | | 34.31 | 6 |
| MOTA | 376 | CB | ILE A | 47 | | 46.333 | | | | 32.16 | 6 |
| ATOM | 377 | CG2 | ILE A | | | 47.346 | | | | 32.65 | 6 |
| ATOM | 378 | CG1 | ILE A | 47 | | 46.504 | 39.32 | | | 38.97 | 6 |
| MOTA | 379 | CD1 | ILE A | 47 | | 47.858 | | | | 28.36 | 6 |
| MOTA | 380 | С | ILE A | 47 | | 46.196 | | | | 26.11 | 8 |
| ATOM | 381 | 0 | ILE A | | | 45.03 | | | | 27.77 | 7 |
| ATOM | 382 | N | LYS A | | | 47.194 | | · | | 25.80 | 6 |
| ATOM | 383 | CA | LYS A | | | 46.985 | | | | 23.91 | 6 |
| ATOM | 384 | CB | LYS A | | | 48.25 | · | | 1.00 | 24.90 | 6 |
| MOTA | 385 | CG | LYS A | | | 48.05 | | - | 1.00 | 26.39 | 6 |
| ATOM | 386 | CD | LYS A | | | 49.23 | | | 9 1.00 | 27.71 | 6 |
| ATOM | 3,87 | CE | LYS A | | | 48.77 | | | 6 1.00 | 32.59 | |
| MOTA | 388 | ΝZ | LYS A | | | 46.59 | | | 4 1.00 | 26.32 | 6 |
| MOTA | 389 | C | LYS A | | | 47.07 | | | 5 1.00 | 27.85 | . 8 |
| ATCM | 390 | 0 | LYS A | | | 45.73 | | 3 54.65 | 3 1.00 | 24.73 | 7 |
| ATOM | 391 | N | SER A | | | 45.29 | | | 5 1.00 | 27.36 | 6 |
| ATOM | 392 | CA | SER A | | | 43.95 | | 19 [™] 53.47 | | 25.04 | 6 |
| MOTA | 393 | CB | SER A | · | | 42.91 | | 9 54.37 | - | 26.94 | 8 |
| ATOM | 394 | OG C | SER A | · | | 46.32 | 2 37.23 | 1 53.29 | | 28.97 | |
| ATOM | 395 396 | 0 | SER A | | | 47.09 | 5 37.88 | 52.61 | 2 1.00 | 31.89 | , |
| MOTA | 396 | • | | | | | | - | | | |
| _ | | | | | | | | | | | |

| | | 46 315 35 879 53.296 1.00 29.71 7 |
|-------|------------------|-----------------------------------|
| | 397 N ARG A 50 | 40.313 33.0.2 |
| ATOM | | 41.41 |
| ATOM | 390 CM 110- 11 | 48.249 34.351 53.318 1.00 26.20 6 |
| MOTA | 333 65 556 | 47 607 33 204 54.172 1.00 22.71 6 |
| MOTA | 400 CG ARG A 50 | 40 010 32 468 54.890 1.00 22.95 6 |
| ATOM | 401 CD ARG A 50 | 40.010 32.400 |
| ATOM_ | 402 NE ARG A 50 | 48.359 31.385 33.762 1.00 16 05 6 |
| | 403 CZ ARG A 50 | 47.708 30.306 33.343 |
| ATOM | 404 NH1 ARG A 50 | 47.430 30.151 34.033 1.05 |
| -TOM | | A7 114 29.303 30.223 2 |
| ATOM | 403 11112 11112 | 46 370 34 051 51.723 1.00 23.30 6 |
| MOTA | 400 0 3444 | 45 319 33 635 52.206 1.00 16.92 8 |
| ATOM | 407 O ARG A 50 | 1 00 21 06 7 |
| ATOM | 408 N PRO A 51 | 40.023 33.020 1 00 00 50 |
| ATOM | 409 CD PRO A 51 | 48.021 34.036 45.765 1.00 32 69 6 |
| | 410 CA PRO A 51 | 46.086 32.633 49.701 1.00 21 57 6 |
| ATOM | 910 0 | 40.002 32.332 |
| ATOM | dir on the | 47.503 33.984 46.352 1.35 |
| ATOM | | 45 353 31 300 50.498 1.00 26./1 b |
| MOTA | 413 0 1110 1 | 47 071 31 066 51.293 1.00 31.32 8 |
| MOTA | 414 O PRO A 51 | 4E 176 30 435 50 250 1.00 40.04 / |
| MOTA | 415 N ALA A 52 | 73,1,7 |
| MOTA | 416 CA ALA A 52 | 45.151 25.122 00.01 42 6 |
| ATOM | 417 CB ALA A 52 | 43.720 20.303 = 200 1 00 26 31 6 |
| | 418 C ALA A 52 | 46.013 28.227 30.000 1.00 30 31 8 |
| ATOM | 419 O ALA A 52 | 45.878 28.239 40.700 1.00 36.00 7 |
| ATOM | 3.0 | 46,909 27.464 50.000 4.00 4.00 |
| ATOM | 420 11 | 47.759 26.578 49.831 1.00 27.52 6 |
| ATOM | 300 | 48 845 25.975 50.717 1.00 26.27 6 |
| ATOM | 422 02 000 | 49 255 25 053 51.641 1.00 29.51 8 |
| MOTA | 423 OG1 THR A 53 | 40.522 27.076 51.502 1.00 24.66 6 |
| ATOM | 424 CG2 THR A 53 | 49.522 27.070 55.00 60 60 6 |
| ATOM | 425 C THR A 53 | 40.900 23.900 10.00 21 98 8 |
| MOTA | 426 O THR A 53 | 45.778 25.226 45.052 1.00.29.62 7 |
| | 427 N LYS A 54 | 47.455 24.782 48.205 1.00 32 62 6 |
| MOTA | 428 CA LYS A 54 | 46./39 23./13 4/.30 |
| ATOM | 420 0 | 47.601 23.151 46.370 1.00 31.99 |
| ATOM | 425 00 000 0 | 46 985 21.967 45.629 1.00 36.62 6 |
| MOTA | 430 CG DIG | 45 733 22 352 44.866 1.00 40.69 |
| ATOM | 431 CD LYS A 54 | 46 059 23 173 43 625 1.00 46 44 6 |
| ATOM | 432 CE LYS A 54 | 46 044 22 393 42 614 1.00 50.68 |
| ATOM | 433 NZ LYS A 54 | 40.044 |
| MOTA | 434 C LYS A 54 | 46.348 22.333 10.330 1.00 34 77 8 |
| ATOM | 435 O LYS A 54 | 45.27/ 21.991 40.330 2100 37 91 7 |
| | 436 N GLU A 55 | 47.216 22.336 49.443 1.00 36 96 6 |
| MOTA | 437 CA GLU A 55 | 46 979 21.290 JU.433 2.00 |
| ATOM | 438 CB GLU A 55 | 40.240 24.400 4 00 47 05 6 |
| MOTA | 450 02 020 | 48.216 19.887 32.133 1.00 |
| MOTA | 777 | 49 552 19.654 52.891 1.00 51.01 6 |
| MOTA | | 49 659 18.688 53.679 1.00 52.65 |
| ATOM | 441 000 000 | 50 407 20 437 52 646 1.00 51.27 8 |
| MOTA | 442 OE2 GLU A 55 | 45 771 21 609 51.322 1.00 34.10 6 |
| ATOM | 443 C GLU A 55 | 43.772 20 769 51 496 1.00 33.08 8 |
| ATOM | 444 O GLUA 55 | 44.002 20.100 1 00 77 70 7 |
| ATOM | 445 N GLU A 56 | 45.723 22.627 51.000 1.00 30 13 6 |
| | 446 CA GLU A 56 | 44.621 23.256 52.755 1.00.25.28 6 |
| ATOM | 447 CB GLU A 56 | 44.824 24.714 33.11 |
| MOTA | 74, 05 05- | 46.204 24.334 33.730 |
| ATOM | | 46 421 26.450 54.181 1.00 30.74 |
| MOTA | 442 05 05 | 46 072 27 369 53.398 1.00 29.77 8 |
| MOTA | 450 OE1 GLU A 56 | 46 060 26 674 55.288 1.00 25.98 8 |
| ATOM | 451 OE2 GLU A 56 | 48.363 20.014 52 024 1.00 29.63 6 |
| ATOM | 452 C GLUA 56 | 43.264 23.114 52.021 1.00 29.90 8 |
| | 453 O GLU A 56 | 42.299 22.384 32.380 1 00 36 76 7 |
| ATOM | 454 N LEU A 57 | 43.188 23.581 50.780 1.00 25 29 6 |
| ATOM | 404 11 220 | 41.944 23.490 50.020 1.00 23.29 6 |
| ATOM | 433 01. 220 | 42.132 24.103 48.629 1.00 22.68 |
| ATOM | 350 02 | 42,402 25.612 48.572 1.00 22.39 5 |
| atom | 457 CG LEU A 57 | 12 554 26 045 47.123 1.00 20.77 6 |
| MOTA | 458 CD1 LEU A 57 | 22.031 26 366 49.156 1.00 17.66 6 |
| ATOM | 459 CD2 LEU A 57 | 41.470 22.037 49.896 1.00 26.02 |
| ATOM | 460 C LEU A 57 | 21.479 22.031 50 014 1.00 23.41 8 |
| ATOM | 461 O LEUA 57 | 40.204 21.732 1 00 24 02 7 |
| A TOM | 462 N LEU A 58 | 42.444 21.143 49.675 1.00 24.82 |

ATOM

75/263 Figure 17-8

| | | | | | | | | | | 49.526 | i.00 2 | 2 44 | 6 |
|------|-----|-----|-------|-----|------|---|-----|-------|--------|--------|--------|---------------------|-----|
| MOTA | 463 | CA | LEU | Α | 58 | | | 194 | 19.718 | | 1.00 2 | | 6 |
| | 464 | | LEU | A | 58 | | 43. | 434 | 19.027 | 48.965 | 1.00 2 | 1.02 | |
| MOTA | | | LEU. | | 58 | | | 838 | 19.471 | 47.558 | 1.00 2 | | 6 |
| MOTA | 465 | | | | 58 | | | 212 | 18.908 | 47.176 | 1.00 2 | 0.35 | 6 |
| MOTA | 466 | | LEU | | | | | 755 | 19.033 | 46.587 | 1.00 2 | 3.28 | 6 |
| ATOM | 467 | | LEU | | 58 | | | | | 50.835 | 1.00 2 | | 6 |
| ATOM | 468 | С | LEU | A | 58 | • | | 797 | 19.054 | | 1.00 2 | | 8 |
| ATOM | 469 | 0 | LEU | Α | 58 | • | 41. | 456 | 17.867 | 50.854 | | | 7 |
| | 470 | | LEU | | 59 | | 41. | 858 | 19.794 | 51.938 | 1.00 2 | 5.44 | |
| ATOM | | - | LEU | | 59 | | 41 | 446 | 19.212 | 53.211 | 1.00 2 | 5.24 | 6 |
| MOTA | 471 | CA | | | 59 | | | 559 | 20.229 | 54.350 | 1.00 2 | 4.68 | 6 |
| ATOM | 472 | CB | LEU | | | | | 956 | 20.490 | 54.912 | 1.00 2 | 7.05 | 6 |
| MOTA | 473 | CG | LEU | | 59 | | | | | 56.001 | 1.00 2 | 4.76 | 6 |
| ATOM | 474 | | LEU | | 59 | | | .912 | 21.565 | | 1.00 2 | | 6 |
| ATOM | 475 | CD2 | LEU | Α | 59 | | | . 492 | 19.184 | 55.474 | | | 6 |
| | 476 | C | LEU | Α | 59 · | | 39 | .991 | 18.807 | 53.045 | 1.00 2 | | |
| ATOM | 477 | ō | LEU | | 59 | | 39 | . 548 | 17.794 | 53.581 | 1.00 2 | | 8 |
| MOTA | | | PHE | | 60 | | | .270 | 19.615 | 52.270 | 1.00 2 | | 7 |
| MOTA | 478 | N | | | | | _ | . 859 | 19.403 | 52.011 | 1.00 2 | 5.00 | 6 |
| ATOM | 479 | CA | PHE | | 60 | | | .054 | 20.560 | 52.605 | 1.00 2 | 6.34 | 6 |
| ATOM | 480 | CB | PHE | | 60 | | | | 20.555 | 52.223 | 1.00 2 | | 6 |
| ATOM | 481 | CG | PHE | Α | 60 | | | .600 | | | | 7.57 | 6 |
| MOTA | 482 | CD1 | PHE | Α | 60 | | | .811 | 19.422 | 52.427 | 1.00 2 | | 6 |
| | 483 | | PHE | | 60 | | 35 | .015 | 21.692 | 51.661 | | | |
| MOTA | 484 | | PHE | | 60 | | 33 | .466 | 19.419 | 52.077 | 1.00 2 | | 6 |
| MOTA | | | PHE | | 60 | | - | .670 | 21.699 | 51.306 | 1.00 2 | 28.08 | 6 |
| MOTA | 485 | | | | | | | .893 | 20.559 | 51.513 | 1.00 2 | 29.48 | 6 |
| MOTA | 486 | CZ | PHE | | 60 | | | .506 | 19.214 | 50.538 | 1.00 2 | 27.78 | 6 |
| MOTA | 487 | С | PHE | A | 60 | | _ | | | 50.158 | 1.00 | 31.57 | 8 |
| ATOM | 488 | 0 | PHE | | 60 | | | .022 | 18.143 | 49.696 | | 26.76 | 7 |
| ATOM | 489 | N | HIS | Α | 61 | | | .734 | 20.220 | | | 28.84 | 6 |
| MOTA | 490 | CA | HIS | | 61 | | 37 | .376 | 20.056 | 48.287 | | | |
| | 491 | CB | HIS | | 61 | | 37 | .365 | 21.405 | 47.561 | | 27.76 | 6 |
| MOTA | 492 | CG | HIS | | 61 | | 36 | .385 | 22.396 | 48.117 | | 30.54 | 6 |
| MOTA | | | HIS | | 61 | | | .056 | 22.549 | 47.907 | | 33.74 | 6 |
| MOTA | 493 | | | | | | | .750 | 23.401 | 48.987 | 1.00 | 34.02 | 7 |
| MOTA | 494 | | HIS | | 61 | | _ | | 24.135 | 49.286 | 1.00 | 32.07 | 6 |
| MOTA | 495 | | HIS | | 61 | | | .691 | | 48.644 | 1.00 | | .7 |
| ATOM | 496 | NE2 | HIS | Α | 61 | | | .649 | 23.638 | 40.044 | 1.00 | | 6 |
| ATOM | 497 | С | HIS | Α | 61 | | | .278 | 19.056 | 47.539 | | | 8 |
| | 498 | 0 | HIS | A | 61 | | 39 | .287 | 18.604 | 48.072 | 1.00 | 25.61 | 7 |
| ATOM | 499 | N | THR | | 62 | | 37 | .895 | 18.705 | 46.310 | 1.00 | | |
| MOTA | | | THR | | 62 | | 3.8 | .658 | 17.749 | 45.488 | | 34.68 | 6 |
| MOTA | 500 | CA | | | 62 | | | .715 | 16.739 | 44.778 | | 34.36 | 6 |
| MOTA | 501 | CB | THR | | | | - | .942 | 17.415 | 43.778 | 1.00 | 34.81 | 8 |
| ATOM | 502 | OG1 | | | 62 | | | | 16.112 | 45.778 | | 34.33 | 6 |
| MOTA | 503 | CG2 | | | 62 | | | .759 | | 44.408 | | 35.60 | 6 |
| MOTA | 504 | С | THR | A | 62 | | | .485 | 18.454 | 43.790 | | 30.85 | 8 |
| ATOM | 505 | 0 | THR | . A | 62 | | | 0.017 | 19.418 | | | 37.38 | 7 |
| MOTA | 506 | N | GLU | Α | 63 | | 4 (| 700 | 17.958 | 44.166 | 1.00 | 37.30 | 6 |
| | 507 | CA | GLU | | 63 | | 4.1 | 1.587 | 18.555 | 43.165 | | 40.68 | |
| MOTA | 508 | CB | GLU | | 63 | | 42 | 2.759 | 17.626 | 42.840 | 1.00 | 43.75 | 6 |
| MOTA | | | CLU | | 63 | | 4 | 3.719 | 17.389 | 43.987 | 1.00 | 50.68 | 6 |
| MOTA | 509 | CG | GLU | | | | | 5.026 | 16.760 | 43.529 | 1.00 | 55.36 | 6 |
| ATOM | 510 | CD | GLU | | 63 | | | 5.789 | 17.441 | 42.808 | 1.00 | 53.03 | 8 |
| ATOM | 511 | | GLU | | 63 | | | | | 43.883 | | 59.56 | 8 |
| ATOM | 512 | OE2 | GLU | I A | 63 | | | 5.285 | 15.585 | | 1.00 | 39.26 | 6 |
| ATOM | 513 | С | GLU | | 63 | | 4 (| 0.894 | 18.939 | 41.860 | | | |
| | 514 | ō | GLU | | 63 | | 4(| 0.771 | 20.116 | 41.535 | | 42.33 | 8 |
| ATOM | | N | ASI | | 64 | | | 0.453 | 17.948 | 41.102 | 1.00 | 37.07 | . 7 |
| MOTA | 515 | | | | | | | 9.782 | 18.224 | 39.845 | | 36.98 | 6 |
| ATOM | 516 | CA | ASI | | 64 | | | 8.957 | 17.000 | 39.426 | 1.00 | 42.19 | 6 |
| MOTA | 517 | CB | ASI | A | 64 | | ٠ د | 8.33/ | | 40.533 | | 47.66 | 6 |
| ATOM | 518 | CG | ASI | • A | 64 | | 3 | 8.037 | 16.501 | | | 47.95 | 8 |
| | 519 | OD: | l ASE | A 9 | 64 | | 3 | 7.039 | 17.193 | 40.851 | | | 8 |
| MOTA | 520 | | 2 ASI | | | | | 8.325 | 15.413 | | | 50.07 | |
| MOTA | | | ASI | | | | | 8.908 | 19.480 | 39.906 | | 33.40 | 6 |
| MOTA | 521 | C | | | | | | 8.927 | | | | 33.64 | 8 |
| atcm | 522 | 0 | | ? A | | | | 8.156 | | | | 30.57 | 7 |
| ATOM | 523 | N | | R A | | | | | | 41.157 | | 29 ⁻ .65 | 6 |
| ATOM | 524 | CA | TY | R A | | | | 7.286 | | | | 30.16 | |
| ATOM | 525 | | TY | R A | 65 | | | 6.300 | | | | 28.49 | |
| | 526 | | | R A | | | | 5.557 | | | | | |
| ATOM | 527 | | 1 TY | | | | 3 | 4.791 | | | | 30.25 | _ |
| ATOM | | | | | | | | 4.126 | | 42.399 | 1.00 | 28.36 | 6 |
| ATOM | 528 | عب | 1 TY | K A | | | _ | | _ | - | | | |

| ATOM | 529 | CD2 | TYR A | . 6 | 55 | | | 638 | | . 181 | 44.15 | | 1.00 2 | 8.28 6.96 | 6 6 |
|--------------|------------|-----------|------------|-----|----------|---|----|-----------------|-----|------------------|--------------|--------------|------------------|----------------|---------|
| ATOM | 530 | CE2 | TYR A | | 55 | | | 980 | | | 44.61 | | 1.00 2 | | 6 |
| ATOM | | CZ | TYR A | | 55 | • | | . 227 . 568 | | .082 .201 | 44.20 | | 1.00 2 | 8.53 | 8 |
| MOTA | 532 | OH | TYR A | | 55 55 | | | . 118 | | .061 | 41.41 | | 1.00 2 | 9.15 | 6 |
| MOTA | 533 | C | TYR A | - | 65 | | | .860 | | .128 | 40.85 | 57 | | 0.45 | 8 |
| ATOM | 534 | 0 N | ILE A | | 66 | | | 122 | | .926 | 42.27 | | 1.00 2 | | 7 |
| MOTA | 535 | CA | ILE A | _ | 66 | | | .986 | 23 | .041 | 42.59 | | 1.00 2 | | 6 |
| ATOM | 536 537 | CB | ILE A | - | 66 | | 40 | .998 | 22 | . 652 | 43.68 | | 1.00 2 | | 6 |
| MOTA MOTA | 538 | CG2 | ILE A | | 66 | | | .009 | | .753 | 43.86 | | 1.00 2 1.00 2 | 1.20 | 6 6 |
| MOTA | 539 | CG1 | ILE A | 4 | 66 | | | .264 | | .341 | 44.99 | 92 | 1.00 2 | | 6 |
| ATOM | 540 | CD1 | ILE A | _ | 66 | | | .478 | 23 | .517 | 45.5 | | 1.00 2 | | 6 |
| ATOM | 541 | С | ILE A | | 66 | | | .761 | | .504 .696 | 41.2 | | 1.00 3 | 1.26 | 8 |
| ATOM | 542 | 0 | ILE F | | 66 | | | .039 .125 | | .559 | 40.5 | | 1.00 2 | | 7 |
| MOTA | 543 | N | ASN A | | 67 67 | | 41 | .902 | 22 | .898 | 39.3 | 37 | 1.00 3 | 0.15 | 6 |
| MOTA | 544 | CA | ASN A | | 67 | | | .563 | 21 | .656 | 38.7 | | | 4.20 | 6 |
| ATOM | 545 546 | CB CG | ASN A | | 67 | | | .712 | 21 | .118 | 39.5 | | 1.00 3 | | 6 |
| ATOM | 547 | | ASN A | | 67 | | 44 | .674 | | .841 | 39.8 | | 1.00 4 | 13.34 37.14 | 8 7 |
| ATOM ATOM | 548 | ND2 | | | 67 | | | .626 | | .845 | 39.9 38.3 | | 1.00 3 | | 6 |
| ATOM | 549 | С | ASN A | | 67 | | | .020 | | .554 | 37.4 | | 1.00 2 | | 8 |
| ATOM | 550 | 0 | ASN A | | 67 | | | .494 | | 3.354 | 38.3 | | 1.00 | | 7 |
| MOTA | 551 | N | THR | | 68 | | | .733 .787 | | 7.791 | 37.4 | | 1.00 2 | 21.75 | 6 |
| MOTA | 552 | CA | THR | | 68 68 | | | .438 | | .111 | 37.5 | 00 | | 16.99 | 6 |
| MOTA | 553 | CB OC1 | THR . | | 68 | | _ | .620 | 21 | 1.695 | 37.3 | | 1.00 | | 8 |
| MOTA | 554 555 | CG2 | | | 68 | | | .549 | 23 | 3.591 | 36.3 | | | 17.59 | 6 |
| ATOM ATOM | 556 | c | THR | | 68 | | | .633 | | 5.263 | 37.7 | | 1.00 | 22.13 21.97 | 6 8 |
| ATOM | 557 | ō | THR | Α | 68 | | | .529 | | 5.088 | 36.8 39.0 | | | 22.32 | 7 |
| MOTA | 558 | N | LEU | A | 69 | | | 3.645 | | 5.582 6.956 | 39.4 | | 1.00 | 23.97 | 6 |
| MOTA | 559 | CA | LEU | | 69 | | | 3.535 3.376 | | 6.982 | 41.0 | | | 24.99 | 6 |
| MOTA | 560 | CB | LEU | | 69 69 | | 37 | 7.023 | | 6.527 | 41.5 | 548 | | 29.08 | 6 |
| MOTA | 561 | CG | LEU LEU | | 69 | | | 7.087 | | 6.416 | 43.0 | 066 | | 30.99 | 6 |
| MOTA | 562 563 | | LEU | | 69 | | 35 | 5.942 | | 7.528 | 41.3 | | | 28.69 | 6 6 |
| ATOM ATOM | 564 | c | LEU | | 69 | | | 772 | | 7.757 | 39.0 38.0 | | 1.00 | 24.90 25.04 | 8 |
| ATOM | 565 | 0 | LEU | | 69 | | | 9.683 | | 8.921 | 39. | | 1.00 | 24.67 | 7 |
| MOTA | 566 | N | MET | | 70 | | | 0.932 2.183 | | 7.128 7.794 | 38. | | | 23.62 | 6 |
| MOTA | 567 | CA | MET | | 70 70 | | | 3.358 | | 6.953 | 39. | | 1.00 | 26.92 | 6 |
| MOTA | 568 | CB CG | MET MET | | 70 | | | 3.418 | | 6.751 | 40. | | 1.00 | 26.69 | 6 |
| MOTA | 569 570 | SD | | A | 70 | | 4 | 4.970 | | 5.929 | 41. | | 1.00 | 30.71 | 16 6 |
| MOTA MOTA | 571 | CE | | A | 70 | | | 6.137 | | 7.077 | 40. | | | 23.20 21.62 | 6 |
| MOTA | 572 | C | MET | Α | 70 | | | 2.324 | | 8.040 | 37. | 982 | | 18.99 | 8 |
| ATOM | 573 | 0 | MET | | 70 | | | 2.903 | | 9.041 | 36. | 632 | | 23.93 | 7 |
| ATOM | 574 | N | GLU | | 71 | | | 1.769 1.859 | _ | 7.204 | 3: | 189 | 1.00 | 24.41 | 6 |
| MOTA | 575 | CA | | | 71 71 | | | 1.681 | | 5.814 | 34 | 582 | 1.00 | 26.22 | 6 |
| ATOM. | 576 | CB | | | 71 | | | 2.224 | | 5.695 | 33. | 167 | 1.00 | 31.75 | 6 |
| MOTA | 577 578 | CG CD | | | 71 | | | 3.737 | _ | 5.905 | | 099 | | 33.00 | 6 |
| MOTA | 579 | | 1 GLU | | 71 | | | 4.288 | 2 | 5.855 | | 983 | | 35.84 | 8 8 |
| MOTA MOTA | 580 | OE | 2 GLU | A | 71 | | | 4.377 | | 6.116 | | 154 | | 30.13 21.86 | 6 |
| ATOM | 581 | C. | GLU | | 71 | | | 0.845 | | 8.160 | | 592 626 | | 21.54 | 8 |
| ATOM | 582 | 0 | GLU | Α | 71 | | | 1.144 | | 28.851 | | 169 | | 19.22 | 7 |
| MOTA | 583 | N | ALA | | 72 | | | 9.649 | | 28.197 29.067 | | 684 | | 19.39 | 6 |
| ATOM | 584 | CA | | | 72 | | | 8.589 7.298 | | 28.743 | | 397 | 1.00 | 19.23 | 6 |
| MOTA | 585 | | | | 72 72 | | | 8.931 | | 30.536 | 34. | . 899 | 1.00 | 26.72 | 6 |
| ATOM | 586 | | ALA ALA | | 72 | | | 8.71 | | 31.383 | 34. | .016 | | 26.12 | 8 7 |
| ATOM | 587 588 | | GLU | | 73 | | 3 | 9.470 |) : | 30.83 | | .079 | | 28.44 | 6 |
| ATOM | 589 | | | | 73 | | | 9.820 | | 32.202 | | .436 | | 29.44 25.84 | 6 |
| ATOM ATOM | 590 | _ | | | 73 | | | 0.15 | | 32.282 | | .931 | | 27.51 | 6 |
| MOTA | 591 | , cc | GLU | Α | 73 | | | 0.64 | | 33.65 | | .349 .841 | | 29.38 | 6 |
| ATOM | 592 | CI | | | 73 | | | 10.84 | 1 | 33.800 33.770 | | .582 | | 32.49 | 8 |
| ATOM | 593 | _ | El GLU | | 73 73 | | | 39.842 41.99 | | 33.77 33.96 | | .277 | | 31.77 | 8 |
| ATOM | 594 | O | E2 GLU | A | 73 | | - | 2 L . J J | - | | • | | | | |
| | | | • | | | | | * | | | | | | | |

| ATOM | 595 596 | | GLU A GLU A | 73 73 | | 0.946 0.859 | 3 | 4.024 | 35.615 35.259 | 1.00 3 1.00 3 | 3.52 | 6 8 |
|------|------------|------|----------------|----------|---|----------------|----------|------------------|------------------|------------------|-------|--------|
| MOTA | 597 | N | ARG A | 74 | 4 | 1.992 | 3 | 2.071 | 35.309 | 1.00 3 | | .7 |
| MOTA | 598 | CA | ARG A | 74 | | 3.128 | . 3 | 2.611 | 34.557 | 1.00 3 | | 6 |
| MOTA | | CB | ARG A | 74 | 4 | 4.405 | | 1.826 | 34.874 | 1.00 3 | | 6 |
| MOTA | 599 | CG | ARG A | 74 | | 4.514 | 3 | 6.467 | 34.205 | 1.00 3 | | 6 |
| MOTA | 600 | | ARG A | 74 | | 5.702 | | 9.714 | 34.754 | 1.00 3 | | 6 |
| MOTA | 601 | CD . | | 74 | | 6.041 | | 8.561 | 33.933 | 1.00 3 | | 7 |
| MOTA | 602 | NE | ARG A | 74 | | 6.646 | | 8.634 | 32.748 | 1.00 3 | 35.55 | 6 |
| MOTA | 603 | CZ | ARG A | 74 | | 6.989 | _ | 9.818 | 32.232 | 1.00 2 | 29.64 | 7 |
| MOTA | 604 | | ARG A | | | 6.906 | | 7.514 | 32.079 | 1.00 | 34.07 | 7 |
| MOTA | 605 | | ARG A | 74 | | 2.894 | | 32.623 | 33.051 | 1.00 2 | 28.61 | 6 |
| MOTA | 606 | C | ARG A | 74 | | 3.431 | • | 33.465 | 32.338 | 1.00 2 | 24.38 | 8 |
| MOTA | 607 | 0 | ARG A | 74 | | 2.107 | | 31.673 | 32.566 | 1.00 2 | | 7 |
| ATOM | 608 | N | CYS A | 75 75 | | 12.107 | | 31.619 | 31.148 | 1.00 | | 6 |
| MOTA | 609 | CA | CYS A | 75 75 | | 11.790 | | 30.167 | 30.682 | 1.00 | | 6 |
| MOTA | 610 | CB | CYS. A | 75 | | 3.281 | | 29.296 | 30.777 | | 37.09 | 16 |
| MOTA | 611 | SG | CYS A | 75 | | 10.489 | | 32.382 | 30.956 | 1.00 | | 6 |
| ATOM | 612 | С | CYS A | 75 | | 10.029 | | 32.598 | 29.834 | 1.00 | | 8 |
| MOTA | 613 | 0 | CYS A | 75 | | 10.023 | | 32.787 | 32.088 | 1.00 | | 7 |
| ATOM | 614 | N | GLN A | 76 | | 39.914 | | 33.575 | 32.144 | 1.00 | | 6 |
| ATOM | 61,5 | CA | GLN A | 76 | | 38.691 | | 34.962 | 31.578 | 1.00 | | 6 |
| MOTA | 616 | CB | GLN A | 76 | | 38.986 | - | 36.064 | 32.094 | 1.00 | | 6 |
| MOTA | 617 | CG | GLN A | 76 | | 38.089 | <i>.</i> | 36.541 | 33.480 | | 41.47 | 6 |
| ATOM | 618 | CD | GLN A | 76 | | 38.479 | | 35.755 | 34.426 | | 45.02 | 8 |
| MOTA | 619 | OE1 | GLN A | | | 38.574 | | 37.846 | 33.606 | | 42.22 | 7 |
| ATOM | 620 | NE2 | | | | 38.703 | _ | | 31.358 | 1 00 | 33.20 | 6 |
| ATOM | 621 | C | GLN A | | | 37.56 | | 32.920 33.598 | 30.760 | | 34.19 | 8 |
| MOTA | 622 | 0 | GLN A | | | 36.73 | | | 31.370 | | 31.81 | 7 |
| ATOM | 623 | N | CYS A | | | 37.522 | | 31.598 | 30.627 | | 31.47 | 6 |
| ATOM | 624 | CA | CYS A | | | 36.51 | | 30.862 | 29.454 | | 30.25 | 6 |
| ATOM | 625 | CB | CYS A | | | 37.18 | | 30.181 29.071 | 30.044 | 1.00 | 33.94 | 16 |
| ATOM | 626 | SG | CYS A | | | 38.47 | | | 31.498 | | 31.97 | 6 |
| ATOM | 627 | C | CAR Y | | | 35.85 | | 29.795 | 32.590 | | 35.15 | 8 |
| ATOM | 628 | Ö | CYS A | | | 36.33 | | 29.503 | 31.018 | | 30.78 | 7 |
| MOTA | 629 | N | VAL A | | | 34.75 | | 29.216 | 31.747 | | 30.55 | 6 |
| MOTA | 630 | CA | VAL A | | | 34.06 | | 28.139 | 31.720 | | 30.06 | 6 |
| ATOM | 631 | CB | VAL A | | | 32.53 | | 28.287 | 32.293 | | 28.23 | 6 |
| ATOM | 632 | CG1 | . VAL A | | | 31.88 | | 27.030 | 32.526 | | 30.67 | 6 |
| ATOM | 633 | CG2 | | | | 32.12 | | 29.503 26.794 | 31.110 | | 29.80 | 6 |
| MOTA | 634 | С | VAL A | | | 34.42 | | 26.422 | 30.077 | | 29.65 | 8 |
| MOTA | 635 | 0 | VAL A | | | 33.85 | | 26.422 | 31.739 | | 28.55 | 7 |
| MOTA | 636 | IJ | PRO A | | | 35.33 | | 26.335 | 33.025 | | 24.39 | 6 |
| MOTA | 637 | CD | PRO A | | | 35.98 | | 24.724 | 31.261 | | 28.89 | 6 |
| ATOM | 638 | CA | PRO A | | | 35.79 | | | 32.434 | 1 00 | 24.49 | 6 |
| MOTA | 639 | CB | PRO A | | | 36.62 | | 24.218 | 32.922 | 1 00 | 25.68 | 6 |
| ATOM | 6 ' 0 | CG | PRO A | | | 37.23 | | 25.500 | 30.881 | 1 00 | 30.13 | 6 |
| ATOM | 6.∡1 | С | PRO 2 | | | 34.66 | | 23.776 | 31.615 | 1 00 | 30.87 | 8 |
| MOTA | 6-2 | 0 | PRO A | | | 33.69 | | 23.624 | 29.727 | 1 00 | 33.44 | 7 |
| ATOM | 643 | N | LYS ? | | | 34.79 | | 23.136 | 29.303 | | 38.52 | _ |
| MOTA | 644 | CA | LYS ? | | | 33.75 | | 22.216 | 28.076 | | 45.18 | 6 |
| MOTA | 645 | CB | LYS ? | 80 A | | 34.20 | | 21.421 | 28.078 | 1 00 | 55.18 | 6 |
| ATOM | 646 | CG | LYS A | | | 35.45 | | 20.589 | | | 60.80 | 6 |
| MOTA | 647 | CD | LYS ? | A 80 | | 35.78 | | 19.827 | 27.000 | | 64.25 | 6 |
| ATOM | . 648 | CE | LYS A | . 80 | | 37.03 | | 18.976 | 27.168 | | 68.95 | 7 |
| ATOM | 649 | NZ | LYS A | . 80 | | 37.36 | | 18.252 | 25.911 | | 36.56 | 6 |
| ATOM | 650 | С | LYS 2 | | | 33.41 | | 21.267 | 30.443 | | 31.61 | 8 |
| MOTA | 651 | ō | LYS | | | 34.29 | | 20.775 | 31.164 | | 32.57 | 7 |
| ATOM | 652 | N | GLY 3 | | | 32.13 | | 21.035 | 30.602 | | 29.81 | 6 |
| ATOM | 653 | CA | | | | 31.63 | | 20.155 | 31.648 | | 28.30 | |
| | 654 | c | GLY . | | | 31.47 | | 20.884 | 32.965 | | | _ |
| ATOM | 655 | ō | GLY | | | 30.54 | | 20.612 | 33.723 | | 25.49 | |
| ATOM | 656 | Ŋ | ALA | | | 32.38 | | 21.830 | 33.218 | | 25.99 | _ |
| MOTA | 657 | CA | | | | 32.3 | 84 | 22.602 | 34.458 | | 26.72 | _ |
| MOTA | 658 | CB | | | | 33.4 | | 23.674 | | · | 22.64 | |
| ATOM | 659 | | ALA . | | | 31.0 | | 23.245 | 34.886 | | 27.84 | _ |
| ATOM | 660 | | ALA | | | 30.7 | | 23.224 | 36.068 | 3 1.00 | 30.00 | , 0 |
| ATOM | 000 | J | - | J | | | | | • | | | |

| | | | | | | | | | | | | 1.00 3 | 1 15 | 7 |
|-------------|-------|-----|-------|----|------|---|-----|--------|---------|-------|-------|--------|--------------------|-----|
| - mow | 661 | N | ARG A | 4 | 83 ' | | 30. | .310 | 23.811 | 33.9 | 51 | 1.00 : | 7.13 | 6 |
| ATOM | 662 | CA | ARG A | | 83 | | 29 | .071 | 24.462 | 34.3 | 45 | 1.00 3 | | |
| ATOM | | | | | 83 | | | . 285 | 24.941 | 33.1 | .27 | 1.00 3 | | 6 |
| ATOM | 663 | CB | ARG A | | | | | . 439 | 26.189 | 33.4 | | 1.00 4 | 2.23 | 6 |
| ATOM | 664 | CG | ARG A | | 83 | | | | 26.020 | 34.5 | | 1.00 4 | | 6 |
| ATOM | 665 | CD | ARG A | | 83 | | | .480 | | 34.9 | | 1.00 5 | | 7 |
| ATOM- | 666 | NE | ARG A | Ą | 83 | | | .904 | 27.303 | | | 1.00 5 | 6 91 | 6 |
| | 667 | CZ | ARG A | | 83 | | 25 | .046 | 27.460 | 36.0 | | 1.00 | 0.04 | 7 . |
| MCTA | | | ARG A | - | 83 | | 24 | .649 | 26.413 | 36.7 | 24 | 1.00 5 | 3.05 | |
| ATOM | 668 | | | | 83 | | | .588 | 28.672 | 36.3 | 04 | 1.00 | 8.03 | 7 |
| ≳TOM | 669 | | ARG | | | | | .208 | 23.531 | 35.1 | | 1.00 3 | 1.50 | 6 |
| ATOM | 670 | С | ARG A | | 83 | | | | 23.749 | 36.3 | | 1.00 2 | 9.62 | 8 |
| ATOM | 671 | 0 | ARG A | A | 83 | | | .056 | 23.743 | 34.3 | | | 3.06 | 7 |
| ATOM | 672 | N | GLU A | Α | 84 | | | .648 | 22.491 | | | 1.00 | | 6 |
| | 673 | CA | GLU . | A | 84 | • | | .819 | 21.568 | 35.3 | | | | 6 |
| MOTA | 674 | CB | GLU . | | 84 | | 26 | .112 | 20.562 | 34.4 | 117 | 1.00 | 7.35 | |
| ATOM | | CG | GLU . | | 84 | | 26 | .989 | 19.684 | 33.4 | 196 | 1.00 | 10.01 | 6 |
| ATOM | 675 | | | | 84 | | 27 | .551 | 20.418 | 32.2 | 267 | 1.00 . | 44.49 | 6 - |
| MOTA | 676 | CD | GLU . | | | | | .925 | 19.723 | 31.3 | 292 | 1.00 | 41.12 | 8 |
| ATOM | 677 | OEl | | | 84 | | | .636 | 21.671 | 32. | | 1.00 | 41.01 | 8 |
| MOTA | 678 | OE2 | GLU | | 84 | | | | 20.823 | 36. | | 1.00 | 35.42 | 6 |
| ATOM | 679 | С | GLU | A | 84 | | | .617 | | 37. | | 1.00 | | 8 |
| ATOM | 680 | 0 | GLU | Α | 84 | | | .246 | 20.816 | | | 1.00 | 35 21 | 7 |
| | 681 | N | LYS | À | 85 | | | .727 | 20.226 | 36. | | 1.00 | 37.22 | 6 |
| ATOM | 682 | CA | LYS | | 85 | , | 29 | .604 | 19.450 | 36. | | 1.00 | 31.93 | |
| ATOM | | | LYS | | 85 | | 3.0 | .841 | 19.030 | 36. | 076 | 1.30 | 40.61 | 6 |
| ATOM | 683 | CB | | | 85 | | | .739 | 17.977 | 36. | 706 | 1.00 | ∔2.63 | 6 |
| ATOM | 684 | CG | LYS | | | | | .038 | 16.640 | | 872 | 1.00 | 45.48 | 6 |
| ATOM | 685 | CD | LYS | | 85 | | | | 15.523 | | | 1.00 | 45.60 | 6 |
| ATOM | 686 | CE | LYS | | 85 | | | .054 | 15.833 | _ | 154 | | 46.16 | 7 |
| MOTA | 687 | NZ | LYS | À | 85 | | | .032 | | | 175 | | 37.56 | 6 |
| ATOM | 688 | С | LYS | A | 85 | | | 0.032 | 20.159 | 30. | 1/3 | | 38.40 | 8 |
| | 689 | ō | LYS | A | 85 | | 30 | 161 (| 19.516 | | 222 | | | 7 |
| MOTA | 690 | Ň | TYR | | 86 | | 3 (| 254 | 21.472 | | 116 | | 35.60 | |
| MOTA | | | TYR | | 86 | • | 3 (| 0.671 | 22.216 | 39. | 307 | | 32.67 | 6 |
| ATOM | 691 | CA | | | 86 | | | 2.151 | 22.610 | | 200 | | 32.09 | 6 |
| ATOM | 692 | CB | TYR | | | | | 3.065 | 21.424 | | 995 | | 33.63 | 6 |
| ATOM | 693 | CG | TYR | | 86 | | | 3.120 | 20.393 | _ | 932 | 1.00 | 32.12 | 6 |
| ATOM | 694 | CD1 | | | 86 | | | | 19.266 | | 723 | | 33.59 | 6 |
| ATOM | 695 | CE1 | TYR | Α | 86 | | | 3.918 | | | 841 | 1 00 | 33.82 | 6 |
| ATOM | 696 | CD2 | TYR | A | 86 | | | 3.839 | 21.306 | | 623 | | 34.55 | 6 |
| ATOM | 697 | CE2 | TYR | Α | 86 | | _ | 4.645 | 20.178 | • | | 1.00 | 32.38 | 6 |
| | 698 | CZ | TYR | | 86 | | 3 | 4.675 | 19.163 | | .566 | 1.00 | 32.30 | 8 |
| ATOM | 699 | OH | TYR | | 86 | | 3 | 5.431 | 18.034 | | .336 | 1.00 | 29.17 | |
| ATOM | | | TYR | | 86 | | 2 | 9.831 | 23.45 | 5 39 | . 597 | | 30.21 | 6 |
| MOTA | 700 | C | TYR | | 86 | | | 0.192 | 24.26 | 5 40 | .445 | | 29.12 | 8 |
| MOTA | 701 | 0 | _ | | 87 | | | 8.712 | 23.59 | 4 38 | . 893 | | 29.44 | 7 |
| ATOM | 702 | N | ASN | | | | | 7.797 | 24.71 | _ | .086 | 1.00 | 28.58 | 6 |
| ATOM | 703 | CA | ASN | | 87 | | | | 24.61 | | .470 | 1.00 | 25.63 | 6 |
| ATOM | 704 | CB | ASN | | 87 | | | 7.154 | | | .596 | | 28.05 | 6 |
| ATOM | 705 | CG | ASN | A | 87 | | | 5.871 | | · . | .672 | | 11.32 | 8 |
| ATOM | 706 | OD: | l ASN | A | 87 | | | 5.275 | | | .072 | | | 7 |
| | 707 | | 2 ASN | | 87 | | | 5.434 | | 5 39 | .506 | 1.00 | .8.35 [3.35 | 6 |
| ATOM | 708 | C | ASN | | 87 | | 2 | 8.580 | 26.01 | | .963 | | | |
| MOTA | | | ASN | | 87 | | | 8.319 | | 1 39 | . 677 | | 32.07 | 8 |
| MOTA | 709 | 0 | | | 88 | | | 9.545 | | | .051 | 1.00 | 32.05 | 7 |
| ATOM | 710 | N | ILE | | | | | 0.407 | | | .809 | 1.00 | 33.77 | 6 |
| ATOM | 711 | CA | | | 88 | | | | | _ | .776 | | 36.13 | 6 |
| ATOM | 712 | CE | ILE | Α | 88 | | | 1.894 | | | .201 | | 37.80 | 6 |
| ATOM | 713 | CG | 2 ILE | A | 38 | | | 2.759 | | | | | 38.92 | 6 |
| | 714 | CG | | | 88 | | | 2.357 | | | .178 | | 41.44 | 6 |
| MOTA | 715 | | 1 ILE | | 88 | | 3 | 2.350 | | | .176 | | . 37.39 . 37.39 | 6 |
| ATOM | | | ILE | | 88 | | | 0.085 | | 7 36 | .482 | | 32.28 | |
| ATOM | 716 | | | | 88 | | | 9.708 | | | .520 | | 32.72 | |
| ATCM | 717 | | ILE | | | | | 30.237 | | | .438 | 3 1.00 | 31.56 | |
| MOTA | 718 | | GLY | | 89 | | | | | | . 207 | | 30.84 | 6 |
| ATOM | 719 | CA | | | 89 | | | 29.994 | | | .09 | | 32.17 | |
| ATOM | 720 | | GLY | | 89 | | | 28.69 | | | | | 30.42 | |
| | 721 | | GL | | 89 | | | 38.628 | | | 1.349 | | 31.51 | |
| ATOM | 722 | | GL | | 90 | | : | 27.67 | 30.29 | | .82 | | | - |
| ATOM | | | | Ä | | | | 26.38 | 7 30.93 | | 5.75 | | 32.92 | |
| ATOM | 723 | | | | | | | 26.31 | | 16 36 | 5.524 | | 34.32 | _ |
| ATOM | . 724 | | | ζÀ | | | | 27.30 | | | 7.12 | | 33.97 | |
| ' ATOM | 725 | | | γA | 90 | | | 25.33. | | _ | 5.50 | | 0 33.88 | 3 7 |
| : COM | 726 | S N | TY | RA | 91 | | | 25.14 | · 26.0 | ` | | | | |

| | | | | | | | | | 27 206 | 1.00 35.76 | 6 |
|---|------|-------|-----|---------|------|-----|--------|----------|----------|--------------|-----|
| | moM | .727 | CA | TYR A | 91 | 24 | .924 | 34.146 | 37.206 | | |
| | | . – | CB | TYR A | 91 | 23 | .465 | 34.589 | 37.058 | 1.00 38.10 | 6 |
| ř | MOT | 728 | | | | | .089 | 35.733 | 37.990 | 1.00 42.40 | 6 |
| Ž | MOTA | 729 | CG | TYR A | 91 | | | 37.057 | 37.688 | 1.00 43.57 | 6 |
| 2 | MOTA | 730 | CD1 | TYR A | 91 | 23 | .417 | | | 1.00 42.44 | 6 |
| | | 731 | CE1 | TYR A | 91 | 23 | .105 | 38.106 | 38.577 | | |
| | MOTA | | | TYR A | 91 | 2.2 | .444 | 35.484 | 39.205 | 1.00 44.07 | 6 |
| i | MOTA | 732 | CD2 | | | | .132 | 36.526 | 40.097 | 1.00 42.67 | 6 |
| 7 | MOTA | 733 | CE2 | TYR A | 91 | | | | 39.775 | 1.00 42.41 | б |
| | MOTA | 734 | CZ | TYR A | 91 | | .462 | 37.825 | 39.773 | | 8 |
| | | 735 | OH | TYR A | 91 | 22 | 2.130 | 38.835 | 40.646 | 1.00 43.69 | |
| | MOTA | | | | 91 | | .242 | 34.082 | 38.701 | 1.00 34.15 | 6 |
| 1 | MOTA | 736 | С | TYR A | | | | 35.014 | 39.266 | 1.00 29.52 | 8 |
| | MOTA | 737 | 0 | TYR A | 91 | | .821 | | 39.333 | 1.00 34.78 | 7 |
| | ATOM | 738 | N | GLU A | 92 | 24 | 1.837 | 32.986 | | | 6 |
| | | 739 | CA | GLU A | 92 | 25 | 5.024 | 32.797 | 40.767 | 1.00 38.46 | |
| | MOTA | | | | | 24 | 1.233 | 31.564 | 41.211 | 1.00 43.99 | 6 |
| | MOTA | 740 | CB | GLU A | | | 3.932 | 31.489 | 42.700 | 1.00 52.10 | 6 |
| | MOTA | 741 | CG | GLU A | | | | | 43.097 | 1.00 58.00 | 6 |
| | ATOM | 742 | CD | GLU A | 92 | | 3.294 | 30.161 | | 1.00 60.63 | 8 |
| | | 743 | | GLU A | | 2 | 4.001 | 29.126 | 43.058 | | |
| | MOTA | | | | | 2 | 2.087 | 30.149 | 43.434 | 1.00 59.58 | 8 |
| | ATOM | 744 | OE2 | GLU A | | | 6.492 | 32.669 | 41.208 | 1.00 36.42 | 6 |
| | ATOM | 745 | С | GLU A | | | | | 42.193 | 1.00 32.92 | 8 |
| | ATOM | 746 | 0 | GLU A | . 92 | | 6.902 | 33.287 | | 1.00 34.12 | 7 |
| | | 747 | N | ASN A | 93 | 2 | 7.280 | 31.883 | 40.473 | 1.00 34.12 | |
| | MOTA | | | ASN A | | 2 | 8.693 | 31.671 | 40.808 | 1.00 33.24 | 6 |
| | ATOM | 748 | CA | | _ | | 8.871 | 30.259 | 41.364 | 1.00 28.52 | 6 |
| | ATOM | 749 | CB | ASN A | | | | 29.859 | 42.299 | 1.00 27.45 | 6 |
| | ATOM | 750 | CG | ASN A | 93 | _ | 7.734 | 29.639 | | 1.00 21.76 | 8 |
| | | 751 | OD1 | ASN A | 93 | | 7.547 | 30.457 | 43.355 | | 7 |
| | MOTA | | | ASN A | | 2 | 6.956 | 28.853 | 41.895 | 1.00 21.79 | |
| | MOTA | 752 . | | | | | 9.529 | 31.843 | 39.535 | 1.00 35.04 | 6 |
| | MOTA | 753 | С | ASN A | | | | | 39.059 | 1.00 33.81 | 8 |
| | MOTA | 754 | 0 | ASN A | 93 | | 0.160 | | 39.010 | 1.00 36.19 | 7 |
| | ATOM | 755 | N | PRO A | 94 | 2 | 9.583 | | | | 6 |
| | | | CD | PRO A | | 2 | 8.970 | 34.231 | 39.690 | 1.00 34.62 | |
| | MOTA | 756 | | | | | 0.274 | | 37.808 | 1.00 34.80 | 6 |
| | ATOM | 757 | CA | PRO A | | | | | 37.791 | 1.00 33.94 | 6 |
| | ATOM | 758 | CB | PRO A | 94 | | 9.924 | | | 1.00 36.13 | 6 |
| | | 759 | CG | PRO A | 94 | | 8.619 | | 38.516 | | 6 |
| | ATOM | 760 | Ċ | PRO P | | . 3 | 1.775 | 33.379 | ·37.733 | 1.00 34.63 | |
| | MOTA | | | | | | 2.443 | | 38.730 | 1.00 34.72 | 8 |
| | ATOM | 761 | 0 | PRO A | | | | | 36.526 | 1.00 33.57 | 7 |
| | MOTA | 762 | N | VAL A | | | 2.299 | | 36.307 | 1.00 30.31 | 6 |
| | MOTA | 763 | CA | VAL A | 3 95 | | 3.735 | 33.499 | | 1.00 29.88 | 6 |
| | | 764 | CB | VAL A | | 3 | 4.085 | 33.171 | 34.841 | | |
| | ATOM | | | _ | | 3 | 5.561 | | 34.574 | 1.00 29.53 | 6 |
| | MOTA | 765 | CG | | | | 3.795 | _ | 34.563 | 1.00 28.05 | 6 |
| | MOTA | 766 | CG2 | 2 VAL 2 | | | | | | 1.00 29.86 | 6 |
| | ATOM | 767 | С | VAL A | a 95 | | 4.195 | | | 1.00 29.07 | 8 |
| | | 768 | 0 | VAL 3 | a 95 | 3 | 3.524 | 35.879 | | | 7 |
| | MOTA | | | SER A | | - | 35.318 | 35.019 | 37.317 | 1.00 30.89 | |
| | MOTA | 769 | N | | | | 5.889 | | | 1.00 32.27 | 6 |
| | MOTA | 770 | CA | SER A | | | | | | 1.00 30.16 | 6 |
| | MOTA | 771 | CB | SER 2 | A 96 | | 34.885 | · | | | 8 |
| | | 772 | OG | SER | a 96 | | 34.600 | 36.545 | | | 6 |
| | ATOM | | c | SER . | | | 37.113 | 1 35.993 | 38.537 | 1.00 32.96 | _ |
| | MOTA | 773 | | | | | 37.60 | | | 1.00 33.77 | 8 |
| | ATOM | 774 | 0 | SER . | | | | | | | 7 |
| | ATOM | 775 | N | TYR A | a 97 | | 37.609 | | | | 6 |
| | | 776 | CA | TYR . | A 97 | | 38.75 | 3 36.712 | | | 6 |
| | ATOM | | CB | | | | 39.83 | g 37.766 | 39.923 | | 0 |
| | ATOM | 777 | | | | | 40.41 | | 38.525 | 1.00 30.39 | 6 |
| | ATOM | 778 | CG | | | | | | | | 6 |
| | MOTA | 779 | CD | 1 TYR | A 97 | | 39.82 | | | | 6 |
| | | 780 | CE | | | | 40.32 | 7 38.358 | 36.178 | | 6 |
| | MOTA | | | | | | 41.53 | 6 36.945 | 38.236 | 1.00 28.43 | |
| | MOTA | 781 | CD | | | | 42.04 | | 36.942 | 1.00 24.73 | . 6 |
| | MOTA | 782 | ÇE | | | | | | | | 6 |
| | MOTA | 783 | CZ | TYR | a 97 | | 41.43 | | | | 8 |
| | | 784 | ОН | | | | 41.91 | | | | |
| | ATOM | | | | | | 38.35 | | 8 41.596 | 1.00 31.10 | |
| | ATOM | 785 | С | TYR | | | | | | | 8 |
| | ATOM | 786 | 0 | TYR | | | 39.17 | - | | | |
| | | 787 | | ALA | | | 37.05 | | | | |
| | MOTA | | | | | | 36.51 | 0 36.24 | 1 43.160 | | |
| | ATOM | 738 | | | | | 35.14 | | 0 43.250 | 1.00 27.71 | |
| | ATOM | -89 | | | | | 36.35 | | | 7 1.00 31.24 | |
| | ATCM | -90 | C | ALA | | | | | | | |
| | | 791 | | ALA | | | 36.33 | | | | _ |
| | ATCM | | | MET | | | 36.24 | 9 34.03 | 0 42.23 | 0 1.00 29.50 | , , |
| | ATOM | 792 | N | LIE I | . ,, | | | | - | | |

| | | V | ET A | 99 | 36.048 | 32.589 | 42.207 | 1.00 29.89 | 6 |
|------|-----|------|-------|-------|--------|---------|--------|------------|-----|
| MOTA | 793 | | | | 35.774 | 32.123 | 40.778 | 1.00 30.48 | 6 |
| ATOM | 794 | | ET A | | | 32.265 | 39.822 | 1.00 29.63 | 6 |
| ATOM | 795 | CG R | ET A | | 36.942 | | | 1.00 29.78 | 16 |
| ATOM | 796 | SD M | ET A | . 99 | 36.426 | 31.939 | 38.126 | | 6 |
| ATOM | 797 | CE M | ET A | . 99 | 35.629 | 30.273 | 38.347 | 1.00 25.05 | |
| | 798 | | ET A | | 37.199 | 31.800 | 42.783 | 1.00 30.81 | 6 |
| ATOM | | | ET A | | 36.993 | 30.757 | 43.406 | 1.00 30.59 | 8 |
| ATOM | 799 | | | | 38.417 | 32.274 | 42.569 | 1.00 32.09 | 7 |
| ATOM | 800 | | | 100 | | 31.557 | 43.114 | 1.00 33.87 | 6 |
| ATOM | 801 | | | 100 | 39.554 | | 42.029 | 1.00 33.95 | 6 |
| ATCM | 802 | C3 ! | HE A | 100 | 40.322 | 30.817 | | | 6 |
| ATOM | 803 | CG I | HE A | 100 | | 29.979 | 42.578 | 1.00 41.14 | |
| | 804 | | | 100 | 41.152 | 28.862 | 43.364 | 1.00 41.84 | 6 |
| MOTA | | | | 100 | 42.768 | 30.339 | 42.372 | 1.00 42.18 | 6. |
| ATOM | 805 | | | 100 | 42.185 | 28.115 | 43.941 | 1.00 41.63 | 6 |
| MOTA | 806 | | | | 43.808 | 29.600 | 42.944 | 1.00 40.50 | 6 |
| MOTA | 807 | | | 100 | 43.517 | 28.487 | 43.729 | 1.00 39.89 | 6 |
| MOTA | 808 | | | 100 | | | 43.895 | 1.00 33.98 | 6 |
| ATOM | 809 | | | 100 | 40.519 | 32.438 | | 1.00 38.21 | 8 |
| ATOM | 810 | | | 100 | 40.706 | 32.231 | 45.088 | 1.00 28.09 | 7 |
| MOTA | 811 | N 1 | THR A | 101 | 41.137 | 33.415 | 43.245 | | |
| | 812 | | | 101 | 42.063 | 34.261 | 43.969 | 1.00 22.19 | 6 |
| ATOM | 813 | | | 101 | 42.623 | 35.378 | 43.072 | 1.00 22.48 | 6 |
| ATOM | | | | A 101 | 43.441 | 34.795 | 42.052 | 1.00 21.99 | , 8 |
| MOTA | 814 | | | | 43.468 | 36.335 | 43.876 | 1.00 15.00 | 6 |
| MOTA | 815 | | | A 101 | | 34.860 | 45.205 | 1.00 21.71 | 6 |
| MOTA | 816 | | | A 101 | 41.408 | | 46.282 | 1.00 23.82 | 8 |
| MOTA | 817 | | | A 101 | 41.988 | 34.845 | 45.068 | 1.00 21.79 | 7 |
| ATOM | 818 | .N | GLY A | A 102 | 40.197 | 35.377 | | 1.00 21.73 | 6 |
| ATOM | 819 | CA | GLY A | A 102 | 39.533 | 35.947 | 46.231 | | |
| ATOM | 820 | С | GLY | A 102 | 39.072 | 34.833 | 47.153 | 1.00 23.03 | 6 |
| | 821 | ō | GLY | A 102 | 39.209 | 34.909 | 48.378 | 1.00 20.41 | 8 |
| ATOM | | | | A 103 | 38.512 | 33.792 | 46.544 | 1.00 22.59 | 7 |
| MOTA | 822 | | | A 103 | 38.028 | 32.640 | 47.276 | 1.00 26.51 | 6 |
| ATOM | 823 | CA | SEK . | A 103 | 37.454 | 31.598 | 46.314 | 1.00 28.10 | 6 |
| ATOM | 824 | CB | SER . | A 103 | | 32.099 | | 1.00 32.01 | 8 |
| MOTA | 825 | | | A 103 | 36.314 | | 48.032 | 1.00 27.73 | 6 |
| MOTA | 826 | | | A 103 | 39.188 | 32.040 | | 1.00 30.61 | 8 |
| ATOM | 827 | O | SER . | A 103 | 39.019 | 31.544 | 49.144 | 1.00 30.01 | 7 |
| ATOM | 828 | 23 | SER . | A 104 | 40.364 | 32.080 | 47.410 | | |
| | 829 | CA | SER | A 104 | 41.590 | 31.552 | 48.008 | 1.00 28.55 | 6 |
| MOTA | 830 | CB | | A 104 | 42.769 | 31.683 | 47.039 | 1.00 28.74 | 6 |
| MOTA | | OG | | A 104 | 42.501 | 31.044 | 45.804 | 1.00 35.04 | 8 |
| ATOM | 831 | | | A 104 | 41.870 | 32.401 | 49.226 | 1.00 25.67 | 6 |
| MOTA | 832 | C | | | 42.026 | 31.897 | 50.338 | 1.00 25.17 | 8 |
| ATOM | 833 | C | SER | A 104 | | .33.705 | 48.986 | 1.00 23.91 | 7 |
| ATOM | 834 | N | LEU | A 105 | 41.909 | | 50.008 | 1.00 23.01 | 6 |
| ATOM | 835 | CA | | A 105 | 42.163 | 34.698 | 49.382 | 1.00 23.57 | 6 |
| ATOM | 836 | CВ | | A 105 | 42.049 | 36.082 | | 1.00 26.30 | 6 |
| ATOM | 837 | CG | LEU | A 105 | 43.158 | 37.091 | 49.672 | | 6 |
| ATOM | 838 | | | A 105 | 44.502 | 36.551 | 49.178 | 1.00 22.38 | |
| | 839 | CD2 | LEII | A 105 | 42.823 | 38.413 | 48.984 | 1.00 27.36 | 6 |
| ATOM | | | 1 211 | A 105 | 41.187 | 34.559 | 51.182 | 1.00 23.48 | |
| ATCM | 840 | C | | | 41.604 | 34.448 | 52.331 | 1.00 21.60 | 8 |
| ATOM | 841 | 0 | LEU | A 105 | 39.887 | 34.556 | 50.897 | | 7 |
| ATOM | 842 | N | ALA | A 106 | | 34.423 | 51.957 | | 6 |
| ATOM | 843 | CA | | A 106 | 38.884 | 34.423 | 51.358 | 1.00 24.28 | |
| ATOM | 844 | CЗ | | A 106 | 37.471 | 34.423 | | | |
| ATOM | 845 | С | ALA | A 106 | 39.088 | 33.158 | 52.790 | | |
| ATOM | 846 | 0 | | A 106 | 38.953 | 33.186 | 54.015 | | |
| | 847 | N | THR | A 107 | 39.410 | 32.057 | 52.111 | | |
| MOTA | | | מעת | A 107 | 39.620 | 30.760 | 52.754 | 1.00 25.54 | |
| MOTA | 848 | CA | | | 39.706 | 29.637 | | 1.00 21.92 | |
| ATOM | 849 | C3 | | A 107 | | 29.688 | | |) 8 |
| ATOM | 850 | OG1 | | A 107 | 38.559 | | | | |
| ATOM | 851 | CG2 | | A 107 | 39.742 | 28.295 | | | |
| ATCM | 852 | C | THR | A 107 | 40.901 | 30.720 | | | |
| | 853 | Ö | THR | A 107 | 40.906 | 30.254 | | | |
| ATOM | 854 | N | GLY. | A 108 | 41.994 | 31.191 | 52.996 | | _ |
| ATOM | | CA | CTV | A 108 | 43.247 | | 53.718 | | |
| ATCM | 855 | | CIV | A 108 | 43.027 | | 55.019 | 1.00 30.26 | |
| ATCM | 856 | C | GLX | A 100 | 43.502 | | | | 3 8 |
| ATCM | 857 | 0 | GLY | A 108 | | | | | |
| ATOM | 858 | N | SER | A 109 | 42.283 | ٥٥.٥٢٥ | | · · · · · | |

Figure 17-14

| ATOM 850 CA SER 2 109 42.002 33.810 56.119 1.00 24.86 6 ATOM 860 CB SER 2 109 41.222 35.898 54.872 1.00 21.07 8 ATOM 861 OG SER 3 109 41.222 35.898 54.872 1.00 21.07 8 ATOM 862 C SER 3 109 41.224 33.214 58.377 1.00 30.92 8 ATOM 863 O SER 4 109 41.224 33.214 58.377 1.00 30.92 8 ATOM 866 CB THR 2 110 49.895 57.721 1.00 24.80 6 ATOM 866 CB THR 3 110 39.676 31.259 57.721 1.00 24.80 6 ATOM 866 CB THR 3 110 39.676 31.259 57.721 1.00 24.80 6 ATOM 866 CB THR 3 110 37.469 31.016 56.669 1.00 30.45 8 ATOM 867 OGI THR 3 110 37.469 31.016 56.669 1.00 30.45 8 ATOM 868 CGZ THR 3 110 37.469 31.016 56.669 1.00 30.45 8 ATOM 869 C THR 3 110 40.712 30.449 58.478 1.00 24.34 6 ATOM 870 OTHR 3 110 40.712 30.449 58.478 1.00 24.34 6 ATOM 871 N VAL 3 111 42.759 29.773 58.416 1.00 22.01 7 ATOM 873 CB VAL 3 111 43.595 28.495 57.391 1.00 25.77 6 ATOM 874 CG1 VAL 3 111 43.595 28.495 57.391 1.00 22.57 6 ATOM 875 CG2 VAL 3 111 43.576 30.071 59.391 1.00 22.57 6 ATOM 876 C VAL 3 111 43.576 30.071 59.391 1.00 22.57 6 ATOM 878 N GLP A 112 44.895 32.100 59.554 1.00 22.67 6 ATOM 878 C GA A 112 44.895 32.100 59.554 1.00 22.67 6 ATOM 878 C GA A 112 44.895 32.100 59.554 1.00 22.67 6 ATOM 880 CB GHA 3 112 44.895 32.100 59.554 1.00 22.67 6 ATOM 880 CB GHA 3 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GHA 3 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.94 7 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.62 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.62 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 24.62 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 31.22 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 31.22 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 31.22 8 ATOM 880 CB GHA 3 112 44.807 32.366 6.837 1.00 31.20 8 AT | | | _ | | | | |
|--|--------|-------------------|---------|----------------------|----------|------------|-----|
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| ## ATOM ## 868 CG2 THR A 110 | | | 37.469 | 31.016 | | | |
| ATOM 869 C THER A 110 40.712 30.282 59.699 1.00 24.74 8 ATOM 870 O THER A 110 40.613 30.282 59.699 1.00 24.74 8 ATOM 871 N VAL A 111 41.715 29.954 57.764 1.00 23.01 7 ATOM 873 CB VAL A 111 41.715 29.954 57.764 1.00 23.01 7 ATOM 873 CB VAL A 111 42.759 29.173 58.416 1.00 24.13 6 ATOM 874 CGI VAL A 111 43.695 28.495 57.391 1.00 22.57 6 ATOM 876 C VAL A 111 43.576 30.071 59.329 1.00 23.14 6 ATOM 877 O VAL A 111 43.576 30.071 59.329 1.00 23.14 6 ATOM 878 N GLN A 112 44.815 27.773 58.121 1.00 22.61 6 ATOM 878 N GLN A 112 44.805 27.773 58.121 1.00 22.51 6 ATOM 879 CA GLN A 112 44.805 32.100 59.554 1.00 22.11 6 ATOM 878 N GLN A 112 44.807 32.100 59.554 1.00 22.12 6 ATOM 880 CB GLN A 112 45.585 33.244 57.330 1.00 28.51 6 ATOM 881 CG GLN A 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 882 CD GLN A 112 46.779 35.219 56.837 1.00 21.10 8 ATOM 883 OPI GLN A 112 44.877 32.316 60.827 1.00 24.62 6 ATOM 886 C GLN A 113 44.877 32.316 60.827 1.00 24.62 6 ATOM 886 C GLN A 113 44.677 32.362 60.827 1.00 24.61 7 ATOM 887 N ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 888 CA ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.915 31.733 62.729 1.00 24.41 7 ATOM 880 CB GLN A 112 44.647 32.362 60.827 1.00 24.62 6 ATOM 880 CB GLN A 112 44.647 32.362 60.827 1.00 24.62 6 ATOM 880 CB GLN A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 880 CB ALA A 113 41.915 31.733 62.729 1.00 24.62 6 ATOM 880 CB ALA A 113 41.916 31.733 62.729 1.00 24.41 7 ATOM 880 CB GLU A 115 44.867 32.816 63.106 1.00 24.49 6 ATOM 889 CB ALA A 113 41.916 31.83 61.224 1.00 19.80 6 ATOM 889 CB ALA A 113 41.916 31.733 62.729 1.00 22.53 8 ATOM 889 CB ALA A 113 41.916 31.733 62.729 1.00 22.53 8 ATOM 889 CB ALA A 113 41.916 31.733 62.729 1.00 22.53 8 ATOM 889 CB GLU A 115 44.867 39.556 63.106 1.00 24.49 6 ATOM 889 CB GLU A 115 44.867 39.556 63.106 1.00 24.99 6 ATOM 899 CD GLU A 115 44.867 39.556 63.106 1.00 24.99 6 ATOM 900 N GLU A 115 44.867 39.556 63.106 1.00 24.99 6 ATOM 901 CC GLU A 115 44.667 39.599 69.790 1.00 22.53 8 ATOM 902 CB GLU A 115 44.667 39.599 69. | | | 38.228 | 29.205 | 58.067 | | |
| ATOM 870 O THIR A 110 40.615 30.282 59.699 1.00 24.74 74 ATOM 871 N VAL A 111 41.715 29.954 57.764 1.00 23.01 8 7 ATOM 872 CA VAL A 111 42.759 29.173 58.416 1.00 24.13 6 7 ATOM 873 CB VAL A 111 43.695 77.773 58.121 1.00 22.51 6 ATOM 876 C VAL A 111 44.895 27.773 58.121 1.00 22.51 6 ATOM 876 C VAL A 111 43.695 28.495 57.391 1.00 23.14 6 ATOM 876 C VAL A 111 43.756 30.071 59.329 1.00 23.14 6 ATOM 876 C VAL A 111 43.760 30.071 59.329 1.00 23.14 6 ATOM 877 O VAL A 111 43.720 29.793 60.518 1.00 24.11 8 ATOM 878 N GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 879 CA GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GLN A 112 45.545 33.224 57.330 1.00 28.51 6 ATOM 881 CG GLN A 112 45.545 33.224 57.330 1.00 28.51 6 ATOM 882 OLG GLN A 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 883 OLG GLN A 112 44.877 14.890 55.694 1.00 29.31 7 ATOM 883 OLG GLN A 112 44.877 14.890 55.694 1.00 29.31 7 ATOM 886 N GL GLN A 112 44.677 31.890 55.694 1.00 29.31 7 ATOM 888 CG GLN A 112 44.677 32.362 60.827 1.00 24.62 6 ATOM 882 CLN A 113 41.914 32.904 61.751 1.00 23.43 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.43 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.43 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.46 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 24.49 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 24.39 7 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.414 7 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.51 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.534 6 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.53 8 ATOM 889 CB ALA A 113 41.914 31.733 62.729 1.00 22.53 8 ATOM 889 CB ALA A 113 41.925 31.930 60.930 60.930 1.00 22.55 8 ATOM 900 CB GLU | | 110 | | 30.449 | 58.478 | 1.00 24.34 | |
| ATOM 871 N VAL A 111 41.715 29.954 57.764 1.00 23.01 7 ATOM 872 CA VAL A 111 42.755 29.1573 58.161 1.00 22.51 6 ATOM 873 CB VAL A 111 43.695 28.495 57.391 1.00 25.77 6 ATOM 875 CG2 VAL A 111 43.695 28.495 57.391 1.00 22.51 6 ATOM 876 C VAL A 111 43.720 29.773 58.121 1.00 22.51 6 ATOM 877 O VAL A 111 43.720 29.793 60.518 1.00 24.11 8 ATOM 878 N GLN A 112 44.895 32.100 59.554 1.00 24.494 7 ATOM 878 N GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 879 CA GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GLN A 112 45.585 33.224 57.330 1.00 28.51 6 ATOM 881 CG GLN A 112 45.789 34.534 55.554 1.00 31.22 8 ATOM 882 CD GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 883 OEI GLN A 112 44.677 32.325 60.827 1.00 24.62 6 ATOM 885 C GLN A 112 44.677 32.326 60.827 1.00 24.62 6 ATOM 886 C GLN A 112 44.677 32.326 60.827 1.00 24.41 8 ATOM 887 N ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 888 CA ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C B ALA A 113 41.915 31.733 62.729 1.00 25.344 6 ATOM 890 C ALA A 113 41.915 31.733 62.729 1.00 25.34 6 ATOM 890 C ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C B GLU A 115 41.669 61.751 1.00 23.33 6 ATOM 890 C B ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C B ALA A 113 41.915 31.733 62.729 1.00 25.34 6 ATOM 890 C B GLU A 115 41.669 61.699 1.00 27.55 8 ATOM 900 N GLU A 115 41.669 61.00 29.90 62.211 1.00 22.53 6 ATOM 900 N GLU A 115 46.699 61.00 29.90 62.211 1.00 22.51 6 ATOM 900 N GLU A 115 46.699 61.00 61.00 1.00 22.51 6 ATOM 901 C C GLU A 115 46.699 61.00 61.00 1.00 22.51 6 ATOM 901 C C GLU A 115 46.699 61.00 61.00 1.00 22.59 8 ATOM 901 C C GLU A 116 45.54 29.264 61.192 1.00 22.59 8 ATOM 901 C C GLU A 116 45.499 61.00 | ATOM | 11A | | 30.282 | 59.699 | | |
| ATOM 871 N NA | ATOM | | | | 57.764 | | |
| ATOM 873 CB VAL A 111 43.695 28.495 57.391 1.00 25.77 6 ATOM 874 CGI VAL A 111 44.845 27.773 58.121 1.00 22.51 6 ATOM 875 CG2 VAL A 111 42.888 27.502 56.534 1.00 22.67 6 ATOM 876 C VAL A 111 43.720 29.793 60.518 1.00 24.11 8 ATOM 877 O VAL A 111 43.720 29.793 60.518 1.00 24.11 8 ATOM 878 N GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 879 CA GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GLN A 112 45.585 33.224 57.330 1.00 28.51 6 ATOM 881 CG GLN A 112 45.789 34.534 56.594 1.00 25.12 6 ATOM 882 CD GLN A 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 883 OEI GLN A 112 44.877 34.890 55.694 1.00 29.13 6 ATOM 884 NEZ CD GLN A 112 A4.877 32.362 60.827 1.00 24.62 6 ATOM 885 C GLN A 112 A4.877 34.890 55.694 1.00 29.13 6 ATOM 886 O GLN A 112 A4.877 34.890 55.694 1.00 29.31 7 ATOM 887 N ALA A 113 A1.91 32.622 60.684 1.00 24.45 6 ATOM 888 CA ALA A 113 A1.91 32.622 60.684 1.00 23.33 6 ATOM 889 CB ALA A 113 A1.91 32.622 60.684 1.00 24.41 7 ATOM 889 CB ALA A 113 A1.91 32.622 60.684 1.00 23.33 6 ATOM 890 C ALA A 113 A1.91 32.622 60.684 1.00 23.33 6 ATOM 891 O ALA A 113 A1.91 31.733 62.729 1.00 23.33 6 ATOM 892 N ILE A 114 A1.867 29.356 63.106 1.00 24.49 6 ATOM 893 CA ILE A 114 A1.867 29.356 63.106 1.00 24.49 6 ATOM 894 CB ILE A 114 A1.902 26.855 63.207 1.00 24.49 6 ATOM 896 CG ILE A 114 A1.902 26.855 63.207 1.00 24.49 6 ATOM 897 CDI ILE A 114 A1.902 26.855 63.207 1.00 24.49 6 ATOM 898 C GLI A 115 A1.867 29.956 63.106 1.00 22.51 6 ATOM 900 N GLU A 115 A6.639 29.992 62.508 1.00 22.51 6 ATOM 901 CA GLU A 115 A6.639 29.992 62.508 1.00 22.51 6 ATOM 902 CB GLU A 115 A6.639 29.992 62.508 1.00 22.51 6 ATOM 903 CG GLU A 115 A6.639 29.992 62.508 1.00 22.53 8 ATOM 904 CD GLU A 115 A6.639 29.992 62.508 1.00 22.53 8 ATOM 907 C GLU A 115 A6.639 29.992 62.508 1.00 22.53 8 ATOM 908 O GLU A 115 A6.639 29.992 62.508 1.00 22.53 8 ATOM 909 N GLU A 116 A6.872 34.982 66.861 1.00 37.26 8 ATOM 910 CA GLU A 116 A6.872 34.982 66.474 1.00 27.56 6 ATOM 910 CA GLU A 116 A6.872 34.982 66.471 1.00 22.53 8 ATOM 910 CA GLU A 116 A6.872 34.982 66.474 | MOTA | | 42 759 | 29 173 | | 1.00 24.13 | 6 |
| ATOM 874 CGI VAL A 111 ATOM 875 CG2 VAL A 111 ATOM 876 C VAL A 111 ATOM 877 O VAL A 111 ATOM 877 O VAL A 111 ATOM 877 O VAL A 111 ATOM 878 N CLN A 112 ATOM 879 CA CLN A 112 ATOM 870 CB GLN A 113 ATO | MOTA | | | | | 1.00 25.77 | 6 |
| ATOM 875 CG2 VAL À 111 42.888 27.502 56.534 1.00 22.67 6 ATOM 876 C VAL À 111 43.760 30.071 59.329 1.00 23.14 6 ATOM 877 0 VAL À 111 43.760 30.071 59.329 1.00 23.14 6 ATOM 878 N GLN À 112 44.895 32.100 59.554 1.00 24.94 7 ATOM 878 N GLN À 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 879 CA GLN À 112 45.585 33.224 57.330 1.00 28.51 6 ATOM 881 CG GLN À 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 882 CD GLN À 112 44.877 34.890 55.694 1.00 29.13 6 ATOM 883 CD GLN À 112 44.877 34.890 55.694 1.00 29.13 6 ATOM 885 C GLN À 112 44.877 34.890 55.694 1.00 29.13 6 ATOM 885 CD GLN À 112 44.877 32.362 60.827 1.00 24.62 6 ATOM 886 O GLN À 112 44.647 32.311 61.939 1.00 21.10 8 ATOM 887 N ALA À 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA À 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA À 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C ALA À 113 41.915 31.733 62.729 1.00 25.34 6 ATOM 891 O ALA À 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 893 CB ALA À 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 893 CB ALA À 113 41.925 31.930 63.946 1.00 27.39 7 ATOM 894 CB ILE À 114 41.867 29.356 63.106 1.00 24.49 6 ATOM 894 CB ILE À 114 41.902 26.855 63.207 1.00 24.49 6 ATOM 896 CG ILE À 114 41.902 26.855 63.207 1.00 24.49 6 ATOM 896 CG ILE À 114 41.902 26.855 63.207 1.00 24.49 6 ATOM 897 CDI ILE À 114 41.902 26.855 63.207 1.00 24.49 6 ATOM 896 CG ILE À 114 41.902 26.855 63.207 1.00 24.49 6 ATOM 896 CG ILE À 114 41.902 26.855 63.207 1.00 24.39 7 ATOM 896 CG ILE À 114 41.902 26.855 63.207 1.00 24.39 6 ATOM 900 N GLU À 115 46.639 29.992 62.508 1.00 22.51 6 ATOM 900 CA GLU À 115 46.639 29.995 62.211 1.00 22.51 6 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.51 6 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.51 6 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.51 6 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.53 8 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.53 8 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.53 8 ATOM 900 CA GLU À 115 46.639 29.995 63.307 1.00 22.53 8 ATOM 900 CA GLU À 115 46.639 29.995 63 | ATOM | | | 20.422 | - | 1.00 22.51 | 6 |
| ATOM 876 C VAL À 111 43.576 30.071 59.329 1.00 23.14 6 ATOM 877 O VAL À 111 43.576 30.071 59.329 1.00 23.14 6 ATOM 878 N GLN A 112 44.101 31.156 58.772 1.00 24.94 7 ATOM 878 N GLN A 112 44.895 32.100 59.554 1.00 25.12 6 ATOM 880 CB GLN A 112 45.545 33.224 57.330 1.00 28.51 6 ATOM 881 CG GLN A 112 45.545 33.224 57.330 1.00 28.51 6 ATOM 883 OEI GLN A 112 45.789 34.514 56.594 1.00 29.13 6 ATOM 883 OEI GLN A 112 45.789 34.514 56.594 1.00 29.13 6 ATOM 884 NE2 GLN A 112 45.789 34.890 55.694 1.00 29.13 6 ATOM 885 C GLN A 112 44.877 34.890 55.694 1.00 29.13 6 ATOM 886 O GLN A 112 44.877 32.362 60.827 1.00 24.62 6 ATOM 887 N ALA A 113 44.647 32.311 61.939 1.00 24.62 6 ATOM 888 CA ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 888 CA ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 27.52 8 ATOM 890 C ALA A 113 41.914 32.904 61.751 1.00 27.52 8 ATOM 891 O ALA A 113 41.915 31.83 61.224 1.00 19.80 6 ATOM 892 N ILE A 114 41.859 30.509 62.211 1.00 24.49 6 ATOM 893 CA ILE A 114 41.857 29.356 63.207 1.00 24.49 6 ATOM 894 CB ILE A 114 41.857 29.356 63.207 1.00 23.346 6 ATOM 895 CGI ILE A 114 41.892 26.855 63.227 1.00 23.46 6 ATOM 896 CGI ILE A 114 41.892 26.855 63.227 1.00 23.46 6 ATOM 897 CDI ILE A 114 41.892 26.855 63.227 1.00 23.46 6 ATOM 898 C GLU A 115 46.639 29.992 62.501 1.00 24.39 6 ATOM 900 N GLU A 115 46.639 29.992 62.508 1.00 22.516 6 ATOM 901 CA GLU A 115 46.639 29.992 62.508 1.00 22.53 8 ATOM 902 CB GLU A 115 46.654 29.560 60.991 1.00 22.39 6 ATOM 903 CG GLU A 115 46.659 29.992 62.508 1.00 22.53 8 ATOM 904 CD GLU A 115 46.654 29.560 60.404 1.00 21.37 6 ATOM 908 O GLU A 115 46.654 29.560 60.404 1.00 21.39 6 ATOM 901 CA GLU A 115 46.654 29.560 60.404 1.00 21.99 6 ATOM 901 CA GLU A 115 46.654 29.560 60.404 1.00 21.99 6 ATOM 903 CG GLU A 115 46.654 29.560 60.404 1.00 21.99 6 ATOM 904 CD GLU A 115 46.654 29.560 60.404 1.00 20.39 6 ATOM 907 C GLU A 115 46.659 29.506 60.404 1.00 20.39 6 ATOM 908 O GLU A 116 47.766 82.660 60.406 60.406 1.00 34.40 6 ATOM 911 CB GLU A 116 47.766 82 | | 874 CG1 VAL A 111 | | | | 1.00 22.67 | 6 |
| ATOM 876 C VAL A 111 43.720 29.793 60.518 1.00 24.19 8 ATOM 878 N GLN A 112 44.101 31.156 58.772 1.00 24.94 7 ATOM 878 N GLN A 112 44.101 31.156 58.772 1.00 24.94 7 ATOM 879 CA GLN A 112 45.082 33.413 58.779 1.00 25.12 6 ATOM 881 CG GLN A 112 45.082 33.413 58.779 1.00 25.14 6 ATOM 882 CD GLN A 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 883 OE1 GLN A 112 46.779 35.219 56.837 1.00 31.22 8 ATOM 884 NEZ GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 O GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 O GLN A 112 44.877 32.321 60.827 1.00 24.62 6 ATOM 886 O GLN A 113 44.877 34.890 55.694 1.00 22.10 8 ATOM 887 N ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C ALA A 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 890 C ALA A 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 891 O ALA A 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 892 C ILE A 114 41.867 29.356 63.271 1.00 24.49 6 ATOM 894 CB ILE A 114 41.867 29.356 63.271 1.00 24.49 6 ATOM 895 CG ILE A 114 41.902 26.855 63.227 1.00 18.97 6 ATOM 896 CG ILE A 114 41.902 26.855 63.227 1.00 18.97 6 ATOM 897 CDI ILE A 114 43.230 29.227 63.757 1.00 22.516 6 ATOM 898 C GGUU A 115 46.639 29.227 63.757 1.00 22.53 6 ATOM 901 CA GLU A 115 46.639 29.227 63.757 1.00 22.53 6 ATOM 903 CG GLU A 115 46.639 29.926 60.016 1.00 22.53 8 ATOM 904 CD GLU A 115 46.639 29.926 60.016 1.00 22.53 8 ATOM 909 N GLU A 115 46.639 29.926 60.016 1.00 22.53 8 ATOM 909 N GLU A 115 46.639 29.926 60.016 1.00 22.53 8 ATOM 901 CA GLU A 115 46.639 29.926 60.016 1.00 22.53 8 ATOM 903 CG GLU A 115 46.639 29.926 60.016 1.00 22.53 6 ATOM 904 CD GLU A 115 46.594 29.264 61.192 1.00 22.55 8 ATOM 909 N GLU A 115 46.594 29.266 60.016 1.00 31.19 7 ATOM 908 O GLU A 115 46.594 29.266 60.016 1.00 31.19 7 ATOM 909 O GLU A 116 44.676 33.959 65.237 1.00 31.90 6 ATOM 911 CB GLU A 116 44.676 33.959 65.237 1.00 31.90 6 ATOM 913 CD GLU A 116 44.676 33.959 60.00 | | 875 CG2 VAL A 111 | | | | 1.00 23.14 | . 6 |
| ATOM 877 O VAL A 111 | | | | | | | 8 |
| ATOM 878 N GLN A 112 44.101 55.15.6 6 ATOM 880 CB GLN A 112 45.082 33.413 58.779 1.00 25.12 6 ATOM 881 CG GLN A 112 45.082 33.413 58.779 1.00 28.51 6 ATOM 882 CD GLN A 112 45.789 34.534 56.594 1.00 29.13 6 ATOM 883 OE1 GLN A 112 46.779 35.219 56.837 1.00 31.22 8 ATOM 884 NEZ GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 65.594 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 65.694 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 65.594 1.00 29.31 7 ATOM 886 OE GLN A 112 44.877 34.890 65.694 1.00 29.31 7 ATOM 887 N ALA A 113 42.813 32.622 60.644 1.00 24.491 7 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C ALA A 113 41.915 31.733 62.279 1.00 25.34 6 ATOM 891 O ALA A 113 41.895 30.509 62.211 1.00 24.49 6 ATOM 893 CA ILE A 114 41.867 29.356 63.106 1.00 24.49 6 ATOM 894 CB ILE A 114 41.524 28.042 62.371 1.00 24.39 7 ATOM 895 CGI ILE A 114 41.922 68.955 63.227 1.00 18.97 6 ATOM 896 CGI ILE A 114 41.922 68.955 63.227 1.00 18.97 6 ATOM 897 O LILE A 114 43.230 29.227 63.757 1.00 22.516 6 ATOM 901 CA GLU A 115 46.639 29.227 63.757 1.00 24.74 8 ATOM 898 C TLE A 114 43.230 29.227 63.757 1.00 24.74 8 ATOM 903 CG GLU A 115 46.639 29.926 64.071 1.00 22.53 6 ATOM 904 CD GLU A 115 46.639 29.926 64.071 1.00 22.53 8 ATOM 905 OEI GLU A 115 46.639 29.926 66.047 1.00 22.53 8 ATOM 906 OEZ GLU A 115 46.639 29.926 66.001 1.00 12.60 8 ATOM 907 C GLU A 115 46.54 29.670 60.044 1.00 22.55 6 ATOM 908 O GLU A 115 46.572 30.006 65.837 1.00 22.53 8 ATOM 909 N GLU A 115 46.572 30.006 65.837 1.00 22.53 8 ATOM 909 N GLU A 115 46.673 30.006 65.837 1.00 22.53 8 ATOM 910 CC GLU A 115 46.673 29.926 64.009 1.00 41.76 8 ATOM 911 CB GLU A 116 44.676 33.959 65.237 1.00 31.99 6 ATOM 910 CC GLU A 116 44.676 33.959 65.237 1.00 31.90 61.00 31.90 61.00 31.90 61.00 31.90 61.00 31.90 61. | | | | | | 1 00 24 94 | |
| ATOM 879 CA GLN À 112 44.895 32.100 39.304 1.00 25.14 6 ATOM 880 CB GLN À 112 45.545 33.244 57.330 1.00 28.51 6 GLN À 112 45.545 33.245 57.330 1.00 28.51 6 GLN À 112 45.545 33.224 57.330 1.00 29.13 6 ATOM 881 CB GLN À 112 45.545 33.224 57.330 1.00 29.13 6 ATOM 882 CD GLN À 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 884 NE2 GLN À 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 885 C GLN À 112 44.877 34.890 55.694 1.00 29.31 7 ATOM 886 C GLN À 112 44.877 32.362 60.827 1.00 24.62 6 ATOM 887 N ALA À 113 42.813 32.622 60.644 1.00 24.41 7 ATOM 887 N ALA À 113 42.813 32.622 60.644 1.00 24.41 7 ATOM 889 CB ALA À 113 40.516 33.183 61.224 1.00 24.39 6 ATOM 890 C ALA À 113 41.991 31.733 62.729 1.00 25.34 6 ATOM 891 C ALA À 113 41.991 31.733 62.729 1.00 25.34 6 ATOM 891 C ALA À 113 41.991 31.733 62.729 1.00 25.34 6 ATOM 893 CA ILE À 114 41.867 29.356 63.106 1.00 24.49 ATOM 893 CA ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 893 CA ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 895 CG2 ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 895 CG2 ILE À 114 41.867 29.356 63.227 1.00 23.46 6 ATOM 895 CG2 ILE À 114 41.867 29.356 63.227 1.00 23.46 6 ATOM 895 CG2 ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 896 CG1 ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 896 CG1 ILE À 114 41.867 29.356 63.227 1.00 24.39 7 ATOM 896 CG1 ILE À 114 43.230 29.27 63.757 1.00 24.74 8 ATOM 896 CG1 ILE À 114 43.230 29.27 63.757 1.00 24.74 8 ATOM 900 N GLU À 115 45.638 29.586 63.017 1.00 24.74 8 ATOM 900 N GLU À 115 45.638 29.586 63.551 1.00 24.99 6 ATOM 900 N GLU À 115 46.639 29.992 62.508 1.00 22.53 8 ATOM 900 CG GLU À 115 46.639 29.992 62.508 1.00 22.53 8 ATOM 900 CG GLU À 115 46.639 29.992 62.508 1.00 22.598 8 ATOM 900 N GLU À 115 46.639 29.992 62.508 1.00 22.598 8 ATOM 900 N GLU À 115 46.639 29.992 62.508 1.00 22.598 8 ATOM 900 N GLU À 115 46.639 29.992 62.508 1.00 22.598 8 ATOM 900 N GLU À 116 44.668 33.999 67.415 1.00 33.40 63. | | 878 N GLN A 112 | | | | | |
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| ATOM 884 NE2 GLN A 112 44.877 32.862 60.827 1.00 24.62 6 ATOM 885 C GLN A 112 44.107 32.362 60.827 1.00 24.62 6 ATOM 886 O GLN A 112 44.107 32.361 61.939 1.00 21.10 8 ATOM 887 N ALA A 113 42.813 32.622 60.644 1.00 23.33 6 ATOM 889 C ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 889 C ALA A 113 41.914 32.904 61.751 1.00 23.33 6 ATOM 890 C ALA A 113 41.915 31.733 62.729 1.00 25.34 6 ATOM 891 O ALA A 113 41.925 31.930 63.946 1.00 27.52 8 ATOM 892 N ILE A 114 41.855 31.930 63.946 1.00 27.52 8 ATOM 893 CA ILE A 114 41.867 29.356 63.106 1.00 24.49 6 ATOM 895 CG2 ILE A 114 41.524 28.042 62.371 1.00 23.46 6 ATOM 895 CG2 ILE A 114 41.902 26.855 63.207 1.00 18.97 6 ATOM 896 CG ILE A 114 40.030 28.015 62.034 1.00 21.17 6 ATOM 897 CD ILE A 114 43.232 29.227 63.757 1.00 24.32 6 ATOM 898 C ILE A 114 43.328 28.817 64.907 1.00 24.74 8 ATOM 899 O N GLU A 115 45.638 29.992 62.508 1.00 22.65 8 ATOM 900 N GLU A 115 45.638 29.992 62.508 1.00 22.65 8 ATOM 901 CA GLU A 115 46.659 29.992 62.508 1.00 22.65 8 ATOM 903 CG GLU A 115 46.659 29.992 62.508 1.00 22.65 8 ATOM 906 OE2 GLU A 115 46.659 29.992 62.508 1.00 22.65 8 ATOM 907 C GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 908 O GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 909 N GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 900 N GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 901 CA GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 903 CG GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 904 CD GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 905 OEI GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 907 C GLU A 115 46.639 29.992 62.508 1.00 22.65 8 ATOM 908 O GLU A 115 46.639 29.999 62.211 1.00 24.74 8 ATOM 908 O GLU A 115 46.639 29.999 62.508 1.00 22.65 8 ATOM 909 N GLU A 115 46.639 29.999 62.508 1.00 22.65 8 ATOM 901 CA GLU A 116 46.637 30.066 64.615 1.00 31.19 7 ATOM 908 O GLU A 115 46.639 29.999 62.508 1.00 22.53 8 ATOM 910 CA GLU A 116 47.002 31.806 66.406 91.00 41.76 8 ATOM 911 CB GLU A 116 47.002 31.806 66.61 1.00 31.19 7 ATOM 918 N PHE A 117 42.577 31.096 67.893 1 | | | 46.779 | | _ | 1.00 31.22 | |
| ATOM 885 C GLN A 112 44.107 32.362 60.827 1.00 21.10 8 ATOM 886 O GLN A 112 44.647 32.311 61.939 1.00 21.10 8 ATOM 887 N ALA A 113 41.914 32.904 61.751 1.00 23.33 61 ATOM 889 CB ALA A 113 41.914 32.904 61.751 1.00 25.34 61 ATOM 889 CB ALA A 113 41.901 31.733 62.729 1.00 25.34 61 ATOM 889 CB ALA A 113 41.901 31.733 62.729 1.00 25.34 61 ATOM 891 O ALA A 113 41.901 31.733 62.729 1.00 25.34 61 ATOM 892 N 1LE A 114 41.859 30.509 62.211 1.00 24.39 7 ATOM 893 CA ILE A 114 41.867 29.356 63.106 1.00 24.49 61 ATOM 894 CB ILE A 114 41.524 28.042 62.371 1.00 23.46 61 ATOM 895 CG2 ILE A 114 41.902 26.855 63.227 1.00 18.97 61 ATOM 896 CG1 ILE A 114 41.902 26.855 63.227 1.00 18.97 61 ATOM 897 CD1 ILE A 114 43.230 29.227 63.757 1.00 24.32 61 ATOM 898 C ILE A 114 43.230 29.580 63.019 1.00 22.51 61 ATOM 899 O ILE A 114 43.230 29.580 63.019 1.00 22.51 61 ATOM 900 N GLU A 115 44.280 29.580 63.019 1.00 24.32 61 ATOM 901 CA GLU A 115 46.639 29.950 63.019 1.00 25.89 61 ATOM 902 CB GLU A 115 46.639 29.950 63.019 1.00 25.89 61 ATOM 903 CG GLU A 115 46.639 29.950 63.019 1.00 22.63 61 ATOM 904 CD GLU A 115 46.639 29.950 63.019 1.00 22.53 61 ATOM 905 OEI GLU A 115 45.638 29.518 63.551 1.00 22.63 61 ATOM 907 C GLU A 115 46.639 29.992 62.508 1.00 22.63 61 ATOM 908 O GLU A 115 46.639 29.992 62.508 1.00 22.63 61 ATOM 909 N GLU A 115 46.639 29.992 64 61.192 1.00 20.39 61 ATOM 909 N GLU A 115 45.724 30.422 64.774 1.00 27.56 61 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 25.98 81 ATOM 908 O GLU A 115 45.724 30.422 64.774 1.00 25.98 61 ATOM 909 N GLU A 116 45.282 32.631 65.705 1.00 35.80 61 ATOM 910 CA GLU A 116 45.434 34.605 64.669 1.00 43.09 61 ATOM 910 CA GLU A 116 45.282 32.631 66.046 1.00 43.09 61 ATOM 911 CB GLU A 116 45.282 32.631 66.061 1.00 34.30 7 ATOM 912 CG GLU A 116 45.282 32.631 66.31 66.04 1.00 43.09 61 ATOM 910 CA GLU A 116 45.434 34.605 64.669 1.00 43.09 61 ATOM 910 CA GLU A 116 45.543 32.238 68.61 1.00 37.26 86 ATOM 911 CB GLU A 116 45.543 32.238 68.61 1.00 37.26 86 ATOM 912 CG GLU A 116 45.543 32.238 66.791 1.00 35.45 60 ATO | | | | 34.890 | | | |
| ATOM 886 O GLN A 112 ATOM 887 N ALA A 113 ATOM 888 CA ALA A 113 ATOM 889 CB ALA A 113 ATOM 889 CB ALA A 113 ATOM 890 C ALA A 113 ATOM 890 C ALA A 113 ATOM 891 O ALA A 113 ATOM 891 O ALA A 113 ATOM 892 N ILE A 114 ATOM 893 CA ILE A 114 ATOM 895 CG2 ILE A 114 ATOM 896 CG1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 898 CG2 ILE A 114 ATOM 899 C ALA 113 ATOM 896 CG1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 898 C ILE A 114 ATOM 899 C ALE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 899 C ILE A 114 ATOM 900 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 903 CG GLU A 115 ATOM 904 CD GLU A 115 ATOM 905 OEI GLU A 115 ATOM 905 OEI GLU A 115 ATOM 906 OE2 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 903 CG GLU A 115 ATOM 904 CD GLU A 115 ATOM 905 OEI GLU A 116 ATOM 907 C GLU A 116 ATOM 908 O GLU A 116 ATOM 909 N GLU A 116 ATOM 910 CA GLU A 116 ATOM 911 CB GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CG GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OEI GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 917 C GLU A 116 ATOM 918 N PHE A 117 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CD PHE A 117 ATOM 922 CB PHE A 117 ATOM 922 CD PHE A 117 ATOM 923 CD2 CCE PHE A 117 ATOM 924 CD2 CCE PHE A 117 ATOM 924 CD | | | | 32.362 | 60.827 | 1.00 24.62 | |
| ATOM 887 N ALA A 113 | | | | 32.311 | 61.939 | | |
| ATOM 888 CA ALA A 113 | | | | | 60.644 | | |
| ATOM 889 CB ALA A 113 | MOTA | | | | 61.751 | 1.00 23.33 | |
| ATOM 899 CB ALA A 113 | ATOM | | | | | | |
| ATOM 890 C ALA A 113 ATOM 891 O ALA A 113 ATOM 892 N ILE A 114 ATOM 893 CA ILE A 114 ATOM 894 CB ILE A 114 ATOM 895 CG2 ILE A 114 ATOM 895 CG2 ILE A 114 ATOM 896 CG2 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 898 C ILE A 114 ATOM 898 C ILE A 114 ATOM 899 O ILE A 114 ATOM 900 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 903 CG GLU A 115 ATOM 904 CG GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 905 OE2 GLU A 115 ATOM 906 OE2 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 906 OE2 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 116 ATOM 910 CA GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CG GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 CB GLU A 116 ATOM 915 CE2 GLU A 116 ATOM 916 CB GLU A 116 ATOM 917 CB GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 919 CA PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 922 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CE2 PHE A 117 ATOM 927 CD2 PHE A 117 ATOM 928 CC1 PHE A 117 ATOM 928 CC1 PHE A 117 ATOM 929 CD2 PHE A 117 ATOM 920 CD3 PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CC1 PHE A 117 ATOM 927 CC2 PHE A 117 ATOM 928 CC1 PHE | ATOM | 889 CB ALA A 113 | | | | 1.00 25.34 | 6 |
| ATOM 891 O ALA A 113 ATOM 892 N ILE A 114 ATOM 893 CA ILE A 114 ATOM 894 CB ILE A 114 ATOM 895 CG2 ILE A 114 ATOM 896 CG1 ILE A 114 ATOM 896 CG1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 898 C ILE A 114 ATOM 898 C ILE A 114 ATOM 899 O ILE A 114 ATOM 900 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 904 CD GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 906 OE2 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 115 ATOM 901 CC GLU A 115 ATOM 901 CC GLU A 115 ATOM 902 CB GLU A 115 ATOM 903 CG GLU A 115 ATOM 904 CD GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 115 ATOM 909 N GLU A 116 ATOM 910 CA GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CG GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CD PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CD2 PHE A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CD2 PHE A 117 ATOM 927 CD2 PHE A 117 ATOM 928 CD2 PHE A 117 ATOM 929 CD2 PHE A 117 ATOM 920 CD3 PHE A 117 ATOM 921 CD2 PHE A 117 ATOM 921 CD2 PHE A 117 ATOM 922 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 ANDREAS ANDRE PROPER A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CD2 PHE A 117 ATOM 927 CD2 PHE A 117 ATOM 928 CD2 PHE A 117 ATOM 929 CD2 PHE A 117 ATOM 929 CD2 PHE A 117 ATOM 920 CD3 PHE A 117 ATOM 921 CD2 PHE A 117 ATOM 922 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ANDREAS ANDRE PASS PASS PASS PASS PASS PASS PASS PAS | ATOM | 890 C ALA A 113 | | | | 1.00 27.52 | 8 |
| ATOM 893 CA ILE A 114 ATOM 894 CB ILE A 114 ATOM 895 CG2 ILE A 114 ATOM 896 CG1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 897 CD1 ILE A 114 ATOM 898 C ILE A 114 ATOM 899 O ILE A 115 ATOM 901 CA GLU A 115 ATOM 902 CB GLU A 115 ATOM 903 CG GLU A 115 ATOM 904 CD GLU A 115 ATOM 905 OE1 GLU A 115 ATOM 906 OE2 GLU A 115 ATOM 907 C GLU A 115 ATOM 908 O GLU A 115 ATOM 909 N GLU A 115 ATOM 901 CA GLU A 115 ATOM 901 CA GLU A 115 ATOM 901 CB GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CB GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 916 CB GLU A 116 ATOM 917 O GLU A 116 ATOM 918 OE2 GLU A 116 ATOM 919 CCB GLU A 116 ATOM 910 CCB GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CB GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 916 CB GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CCB PHE A 117 ATOM 919 CCB PHE A 117 ATOM 910 CB PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CB PHE A 117 ATOM 921 CB PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CEI PHE A 117 ATOM 927 CCB PHE A 117 ATOM 928 CD2 PHE A 117 ATOM 929 CCB PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CB PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 ATOM 925 CD2 PHE A 117 ATOM 926 CCEI PHE A 117 ATOM 927 ATOM 928 CCEI PHE A 117 ATOM 9294 CCEI PHE A 117 ANDOM 9294 CCEI | MOTA | 891 O ALA A 113 | | | | 1.00 24.39 | 7 |
| ATOM 893 CA ILE A 114 41.524 28.042 62.371 1.00 23.46 6 ATOM 895 CG2 ILE A 114 41.902 26.855 63.227 1.00 18.97 6 ATOM 896 CG1 ILE A 114 40.030 28.015 62.034 1.00 21.17 6 ATOM 897 CD1 ILE A 114 40.030 28.015 62.034 1.00 21.17 6 ATOM 898 C ILE A 114 43.230 29.227 63.757 1.00 24.32 6 ATOM 899 O ILE A 114 43.230 29.227 63.757 1.00 24.32 6 ATOM 900 N GLU A 115 45.638 29.518 63.551 1.00 25.89 6 ATOM 901 CA GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 902 CB GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 904 CD GLU A 115 46.554 29.264 61.192 1.00 20.39 6 ATOM 905 OE1 GLU A 115 47.668 29.670 60.244 1.00 21.39 6 ATOM 906 OE2 GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 907 C GLU A 115 46.73 30.006 65.837 1.00 22.53 8 ATOM 908 O GLU A 115 46.73 30.006 65.837 1.00 22.53 8 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 910 CA GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 911 CB GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 912 CG GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 913 CD GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 914 OE1 GLU A 116 45.434 34.605 64.069 1.00 41.74 8 ATOM 915 CE2 GLU A 116 45.434 34.605 64.069 1.00 41.14 6 ATOM 916 C GLU A 116 45.434 34.605 64.069 1.00 41.76 8 ATOM 916 C GLU A 116 45.434 34.605 64.069 1.00 41.76 8 ATOM 917 O GLU A 116 45.543 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 35.80 6 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 35.80 6 ATOM 910 CA PHE A 117 42.577 31.096 67.893 1.00 35.80 6 ATOM 920 CB PHE A 117 42.577 31.096 67.893 1.00 35.80 6 ATOM 921 CG PHE A 117 42.577 31.096 67.893 1.00 35.80 6 ATOM 922 CD1 PHE A 117 40.383 29.979 68.833 1.00 37.14 6 ATOM 922 CD2 PHE A 117 40.385 30.549 70.323 1.00 35.80 6 | | 892 N ILE A 114 | | | | 1.00 24.49 | 6 |
| ATOM 894 CB ILE A 114 41.524 28.025 63.227 1.00 18.97 6 ATOM 895 CG2 ILE A 114 41.902 26.855 63.227 1.00 18.97 6 ATOM 896 CG1 ILE A 114 40.030 28.015 62.034 1.00 21.17 6 ATOM 897 CD1 ILE A 114 43.230 29.227 63.757 1.00 24.32 6 ATOM 898 C ILE A 114 43.230 29.227 63.757 1.00 24.32 6 ATOM 899 O ILE A 114 43.328 28.817 64.907 1.00 24.74 8 ATOM 900 N GLU A 115 44.280 29.580 63.019 1.00 26.58 7 ATOM 901 CA GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 902 CB GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 903 CG GLU A 115 46.554 29.264 61.192 1.00 20.39 6 ATOM 905 OE1 GLU A 115 17.668 29.670 60.244 1.00 21.39 6 ATOM 905 OE1 GLU A 115 18.362 28.769 59.722 1.00 22.53 8 ATOM 906 OE2 GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 907 C GLU A 115 46.173 30.006 65.837 1.00 25.98 8 ATOM 908 O GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 910 CA GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 912 CG GLU A 116 45.434 34.605 64.069 1.00 41.14 6 ATOM 913 CD GLU A 116 45.872 34.982 64.420 1.00 43.09 6 ATOM 914 OE1 GLU A 116 45.872 34.982 64.420 1.00 43.09 6 ATOM 915 CE2 GLU A 116 45.872 34.982 66.761 1.00 37.26 8 ATOM 916 C GLU A 116 45.434 34.605 64.069 1.00 41.14 6 ATOM 917 O GLU A 116 45.872 34.982 66.761 1.00 35.11 6 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 35.45 6 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 67.800 920 CB PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 921 CG PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 | | 893 CA ILE A 114 | | | | 1 00 23.46 | |
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| ATOM 896 CG1 ILE A 114 39.598 26.791 61.239 1.00 22.51 6 ATOM 897 CD1 ILE A 114 43.230 29.227 63.757 1.00 24.32 6 ATOM 900 N GLU A 115 45.638 29.518 63.551 1.00 25.89 6 ATOM 902 CB GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 904 CD GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 905 OE1 GLU A 115 47.668 29.670 60.244 1.00 21.39 6 ATOM 906 OE2 GLU A 115 47.848 30.887 60.016 1.00 19.60 8 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 908 O GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 909 N GLU A 115 46.173 30.006 65.837 1.00 25.98 8 ATOM 909 N GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 910 CA GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 912 CG GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 913 CD GLU A 116 45.884 34.605 64.420 1.00 41.14 6 ATOM 913 CD GLU A 116 45.884 34.982 64.420 1.00 41.14 6 ATOM 913 CD GLU A 116 45.884 34.982 64.420 1.00 43.09 6 ATOM 915 OE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 917 O GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 917 O GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 917 O GLU A 116 47.802 34.369 63.849 1.00 37.26 8 ATOM 917 O GLU A 116 45.543 32.131 66.947 1.00 35.11 6 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 37.14 6 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 37.14 6 ATOM 920 CB PHE A 117 42.577 31.096 67.893 1.00 37.14 6 ATOM 921 CG PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 922 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.920 1.00 35.80 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | 895 CG2 ILE A 114 | | | | | |
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| ATOM 900 N GLU A 115 45.638 29.518 63.551 1.00 25.89 6 ATOM 901 CA GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 903 CG GLU A 115 46.639 29.992 62.508 1.00 22.63 6 ATOM 903 CG GLU A 115 46.639 29.992 62.508 1.00 20.39 6 ATOM 904 CD GLU A 115 47.668 29.670 60.244 1.00 21.39 6 ATOM 905 OE1 GLU A 115 47.848 30.887 60.016 1.00 19.60 8 ATOM 906 OE2 GLU A 115 18.362 28.769 59.722 1.00 22.53 8 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 908 O GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 910 CA GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 911 CB GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 912 CG GLU A 116 44.676 33.959 65.237 1.00 36.91 6 ATOM 913 CD GLU A 116 44.676 33.959 65.237 1.00 36.91 6 ATOM 914 OE1 GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 915 OE2 GLU A 116 47.072 35.886 65.267 1.00 43.42 8 ATOM 916 C GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 917 O GLU A 116 44.543 32.131 66.947 1.00 35.11 6 ATOM 918 N PHE A 117 43.343 31.598 66.761 1.00 37.26 8 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 919 CA PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 920 CB PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | | | | | | |
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| ATOM 902 CB GLU A 115 46.639 29.926 61.192 1.00 20.39 6 ATOM 903 CG GLU A 115 47.668 29.670 60.244 1.00 21.39 6 ATOM 905 OE1 GLU A 115 47.848 30.887 60.016 1.00 19.60 8 ATOM 906 OE2 GLU A 115 18.362 28.769 59.722 1.00 22.53 8 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 908 O GLU A 115 46.173 30.006 65.837 1.00 25.98 8 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 910 CA GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 44.676 33.959 65.237 1.00 36.91 6 ATOM 912 CG GLU A 116 46.872 34.982 64.420 1.00 43.42 8 ATOM 913 CD GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 914 OE1 GLU A 116 47.072 35.886 65.267 1.00 43.42 8 ATOM 915 OE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 916 C GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 35.41 6 ATOM 919 CA PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 920 CB PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | | 45.638 | | | | |
| ATOM 903 CG GLU A 115 46.554 29.670 60.244 1.00 21.39 6 ATOM 904 CD GLU A 115 47.668 29.670 60.244 1.00 21.39 6 ATOM 905 OE1 GLU A 115 47.848 30.887 60.016 1.00 19.60 8 ATOM 906 OE2 GLU A 115 18.362 28.769 59.722 1.00 22.53 8 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 908 O GLU A 115 46.173 30.006 65.837 1.00 25.98 8 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 910 CA GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 45.434 34.605 64.069 1.00 41.14 6 ATOM 912 CG GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 913 CD GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 914 OE1 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 915 OE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 916 C GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 35.45 6 ATOM 920 CB PHE A 117 42.577 31.096 67.893 1.00 37.14 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 | | | 46.639 | | | 1.00 22.03 | |
| ATOM 904 CD GLU A 115 47.668 29.670 60.244 1.00 21.39 8 ATOM 905 OE1 GLU A 115 47.848 30.887 60.016 1.00 19.60 8 ATOM 906 OE2 GLU A 115 18.362 28.769 59.722 1.00 22.53 ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 908 O GLU A 115 45.724 30.422 64.774 1.00 27.56 6 ATOM 909 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 910 CA GLU A 116 45.267 31.660 64.615 1.00 31.19 7 ATOM 911 CB GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 46.676 33.959 65.237 1.00 36.91 6 ATOM 912 CG GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 913 CD GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 914 OE1 GLU A 116 47.072 35.886 65.267 1.00 43.42 8 ATOM 915 CE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 916 C GLU A 116 45.434 32.131 66.947 1.00 35.11 6 ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 920 CB PHE A 117 40.383 39.979 68.533 1.00 37.14 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | | 46.554 | 29.264 | | | |
| ATOM 905 OE1 GLU A 115 | | | 47 660 | 29.670 | 00.24. | | - |
| ATOM 905 OE2 GLU A 115 18.362 28.769 59.722 1.00 22.53 8 4 4 5 7 7 8 7 8 8 9 8 9 8 9 8 9 8 9 8 9 8 9 8 | | | | | 60.016 | 1.00 19.60 | |
| ATOM 907 C GLU A 115 45.724 30.422 64.774 1.00 27.56 6 8 8 8 8 8 9 9 9 9 8 0 GLU A 115 46.173 30.006 65.837 1.00 25.98 8 8 8 9 9 9 9 N GLU A 116 45.267 31.660 64.615 1.00 31.19 7 9 9 9 N GLU A 116 45.282 32.631 65.705 1.00 35.80 6 8 9 11 CB GLU A 116 44.676 33.959 65.237 1.00 36.91 6 8 9 11 CB GLU A 116 45.434 34.605 64.069 1.00 41.14 6 9 12 CG GLU A 116 46.872 34.982 64.420 1.00 43.09 6 9 13 CD GLU A 116 46.872 34.982 64.420 1.00 43.09 6 9 14 OE1 GLU A 116 47.072 35.886 65.267 1.00 43.42 8 9 14 OE1 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 9 15 CE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 9 15 CE2 GLU A 116 45.054 32.131 66.947 1.00 35.11 6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 | | 905 OEI GLO A 115 | | | | 1.00 22.53 | |
| ATOM 908 O GLU A 115 | atom | | | | 64.774 | 1.00 27.56 | 6 |
| ATOM 909 N GLU A 116 | MOTA | | | | | 1.00 25.98 | 8 |
| ATOM 910 CA GLU A 116 45.282 32.631 65.705 1.00 35.80 6 ATOM 911 CB GLU A 116 44.676 33.959 65.237 1.00 36.91 6 ATOM 912 CG GLU A 116 45.434 34.605 64.069 1.00 41.14 6 ATOM 913 CD GLU A 116 46.872 34.982 64.420 1.00 43.09 6 ATOM 914 OE1 GLU A 116 47.072 35.886 65.267 1.00 43.42 8 ATOM 915 OE2 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 916 C GLU A 116 44.543 32.131 66.947 1.00 35.11 6 ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 43.343 31.598 66.761 1.00 34.30 7 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 920 CB PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | MOTA | | | | | 1.00 31.19 | |
| ATOM 910 CA GLU A 116 ATOM 911 CB GLU A 116 ATOM 912 CG GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | MOTA | 909 N GLU A 116 | | | | 1.00 35.80 | 6 |
| ATOM 911 CB GLU A 116 ATOM 912 CG GLU A 116 ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 CE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | | | | | · | 1.00 36.91 | 6 |
| ATOM 912 CG GLU A 116 45.434 34.982 64.420 1.00 43.09 6 ATOM 913 CD GLU A 116 47.072 35.886 65.267 1.00 43.42 8 ATOM 914 OE1 GLU A 116 47.802 34.369 63.849 1.00 41.76 8 ATOM 915 CE2 GLU A 116 47.802 34.369 63.849 1.00 35.11 6 ATOM 916 C GLU A 116 44.543 32.131 66.947 1.00 35.11 6 ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 ATOM 918 N PHE A 117 43.343 31.598 66.761 1.00 34.30 7 ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 920 CB PHE A 117 41.300 30.399 67.415 1.00 35.45 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | 911 CB GLU A 116 | | | | | |
| ATOM 913 CD GLU A 116 ATOM 914 OE1 GLU A 116 ATOM 915 OE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | | 912 CG GLU A 116 | | | | | 6 |
| ATOM 914 OE1 GLU A 116 ATOM 915 CE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | | 913 CD GLU A 116 | | | | | |
| ATOM 915 CE2 GLU A 116 ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | | 914 OE1 GLU A 116 | | | | | 8 |
| ATOM 916 C GLU A 116 ATOM 917 O GLU A 116 ATOM 918 N PHE A 117 ATOM 919 CA PHE A 117 ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 | | | 47.802 | | | | |
| ATOM 917 O GLU A 116 45.054 32.228 68.061 1.00 37.26 8 7 7 7 7 8 7 8 7 8 7 8 7 8 7 8 8 8 8 | | | 44.543 | | | / | ٥ |
| ATOM 918 N PHE A 117 43.343 31.598 66.761 1.00 34.30 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 | | | | 32.22 | · | | - |
| ATOM 919 CA PHE A 117 42.577 31.096 67.893 1.00 34.44 5 ATOM 920 CB PHE A 117 41.300 30.399 67.415 1.00 35.45 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | 4 4 7 | | | g 66.761 | | , |
| ATOM 920 CB PHE A 117 41.300 30.399 67.415 1.00 35.45 6 ATOM 921 CG PHE A 117 40.383 29.979 68.533 1.00 37.14 6 ATOM 922 CD1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 ATOM 923 CD2 PHE A 117 40.196 28.630 68.832 1.00 41.05 6 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | | | | | | 1.00 34.44 | 5 |
| ATOM 920 CB PHE A 117 ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | atom | | | | | 1.00 35.45 | |
| ATOM 921 CG PHE A 117 ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 39.705 30.930 69.290 1.00 35.80 6 40.196 28.630 68.832 1.00 41.05 6 38.853 30.549 70.323 1.00 38.08 6 | ATOM | | | | | 1.00 37.14 | |
| ATOM 922 CD1 PHE A 117 ATOM 923 CD2 PHE A 117 ATOM 924 CE1 PHE A 117 38.853 30.549 70.323 1.00 38.08 6 | ATOM | 921 CG PHE A 11/ | | | | 1.00 35.80 | |
| ATOM 923 CD2 PHE A 117 40.150 20.549 70.323 1.00 38.08 6 | | | | | | 1.00 41.05 | _ |
| 38.833 30.343 | | 117 | | | | | 6 |
| | | 924 CE1 PHE A 117 | . 50.65 | , ,,,,, , | • | | |

| | | • | • | | | | | _ |
|--------|-------|----------------|---|--------|---------|---------|--------------|-----|
| | | nur : 117 | | 39.338 | 28.234 | 69.874 | 1.00 40.44 | 6 |
| ATOM | 925 C | E2 PHE A 117 | | | 29.198 | 70.617 | 1.00 38.64 | 6 |
| ATOM | 926 C | Z PHE A 117 | | 38.668 | | | | 6 |
| | | | | 43.424 | 30.094 | 68.669 | 1.00 34.24 | |
| ATOM | 927 | | | | 30.136 | 69.898 | 1.00 33.54 | 8 |
| MCTA | 928 | PHE A 117 | | 43.490 | | | | 7 |
| | | 110 | | 44.069 | 29.194 | 67.933 | 1.00 33.14 | |
| MCTA | 929 N | | | 44.898 | 28.158 | 68.523 | 1.00 32.62 | 6 |
| ATOM- | 930 | CA LEU A 118 | | | | | 1.00 30.59 | 6 |
| | | CB LEU A 118 | | 45.155 | 27.056 | 67.488 | 1.00 30.33 | |
| MOTA | | | | 43.900 | 26.297 | 67.038 | 1.00 27.87 | 6 |
| ATOM ' | 932 (| CG LEU A 118 | | | | 65.996 | 1.00 20.81 | 6 |
| ATOM | 933 (| CD1 LEU A 118 | | 44.244 | 25.232 | | | 6 |
| | | CD2 LEU A 118 | | 43.259 | 25.662 | 68.257 | 1.00 28.37 | |
| ATOM | - | D2 110 R 110 | | 46.216 | 28.696 | 69.084 | 1.00 34.37 | 6 |
| ATOM | 935 (| C LEU A 118 | | | | 69.708 | 1.00 36.15 | 8 |
| ATOM | 936 (| O LEU A 118 | | 46.983 | 27.964 | | 1.00 34.75 | 7 |
| | | | | 46.481 | 29.974 | 68.843- | | |
| MOTA | | | | 47.679 | 30.609 | 69.365 | 1.00 34.34 | 6 |
| ATOM | 938 (| CA LYS A 119 | | | 31.739 | 68.448 | 1.00 33.52 | 6 |
| ATOM | 939 (| CB LYS A 119 | | 48.143 | | | 1.00 37.98 | 6 - |
| | | CG LYS A 119 · | | 48.614 | 31.270 | 67.100 | | |
| ATOM | • | **** 3 110 | | 49.111 | 32.430 | 66.263 | 1.00 43.40 | 6 |
| ATOM | 941 | CD LYS A 119 | | | 31.928 | 64.949 | 1.00 46.52 | 6 |
| ATOM | 942 | CE LYS A 119 | | 49.691 | | | 1.00 51.48 | 7 |
| | - | NZ LYS A 119 | | 50.167 | 33.050 | 64.092 | 1.00 31.40 | 6 |
| MOTA | | | | 47.273 | 31.191 | 70.705 | 1.00 34.85 | |
| ATOM | - | C LYS A 119 | | 48.112 | 31.465 | 71.562 | 1.00 38.12 | 8 |
| MOTA | 945 | O LYS A 119 | | | | 70.869 | 1.00 34.15 | 7 |
| | 946 | N GLY A 120 | | 45.967 | 31.372 | | | 6 |
| MOTA | - | | | 45.431 | 31.927 | 72.094 | 1.00 36.25 | |
| ATOM | | | | 44.860 | 33.310 | 71.851 | 1.00 39.02 | 6 |
| ATOM | 948 | C GLY A 120 | | | | 72.796 | 1.00 46.23 | 8 |
| ATOM | 949 | O GLY A 120 | | 44.640 | 34.072 | | 1.00 30.40 | 7 |
| | | N ASN A 121 | | 44.619 | 33.644 | 70.586 | 1.00 38.48 | |
| MOTA | | N ASN A ILI | | 44.079 | 34.956 | 70.247 | 1.00 37.47 | 6 |
| MCTA | 951 | CA ASN A 121 | | _ | 35.530 | 69.170 | 1.00 39.57 | 6 |
| ATOM | 952 | CB ASN A 121 | | 44.928 | 35.624 | | 1.00 41.81 | 6 |
| | 953 | CG ASN'A 121 | | 46.340 | 35.871 | 69.622 | | |
| ATOM | 955 | co ASN A 101 | | 47.078 | 34.938 | 69.926 | 1.00 47.67 . | 8 |
| MOTA | 954 | OD1 ASN A 121 | | | 37.134 | 69.675 | 1.00 43.63 | 7 |
| ATOM | 955 | ND2 ASN A 121 | | 46.727 | | | 1.00 36.59 | 6 |
| | 956 | C ASN A 121 | | 42.637 | 34.893 | 69.772 | 1.00 30.33 | |
| MOTA | | | | 42.037 | 33.818 | 69.704 | 1.00 34.08 | 8 |
| MOTA | 957 | O ASN A 121 | | 42.092 | 36.061 | 69.446 | 1.00 33.53 | 7 |
| ATOM | 958 | N VAL A 122 | | | | 68.976 | 1.00 34.77 | 6 |
| | 959 | CA VAL A 122 | | 40.720 | 36.166 | | 1.00 32.70 | 6 |
| ATOM | | 400 | | 39.861 | 37.064 | 69.898 | 1.00 38.20 | |
| ATOM | 960 | CB VAL A 122 | | 38.418 | 37.096 | 69.388 | 1.00 37.55 | 6 |
| ATOM | 961 | CG1 VAL A 122 | | | | 71.342 | 1.00 37.77 | 6. |
| ATOM | 962 | CG2 VAL A 122 | | 39.918 | 36.553 | | 1.00 31.08 | 6 |
| | 963 | C VAL A 122 | | 40.731 | 36.781 | 67.596 | 1.00 31.00 | |
| ATOM | | | | 40.991 | 37.967 | 67.441 | 1.00 34.19 | 8 |
| ATOM | 964 | 0 VAL A 122 | | 40.451 | 35.975 | 66.588 | 1.00 31.14 | 7 |
| ATOM | 965 | N ALA A 123 | | | | 65.231 | 1.00 30.26 | 6 |
| ATOM | 966 | CA ALA A 123 | | 40.451 | 36.476 | 54.227 | 1.00 32.14 | 6 |
| | | CB ALA A 123 | | 41.307 | 35.588 | 64.327 | 1.00 32.14 | |
| ATOM | 967 | CD 7444 11 122 | | 39.038 | 36.533 | 64.716 | 1.00 28.26 | 6 |
| MCTA | 968 | C ALA A 123 | | | 35.924 | 65.281 | 1.00 29.28 | , 8 |
| ATOM | 969 | O ALA A 123 | | 38.132 | | 62.621 | 1.00 28.70 | 7 |
| | 970 | N PHE A 124 | | 38.875 | 37.276 | 63.631 | 1.00 20.70 | 6 |
| ATOM | | | | 37.601 | 37.475 | 62.976 | 1.00 28.38 | |
| ATOM | 971 | CA PHE A 124 | | 36.920 | | 63.563 | 1.00 29.16 | 6 |
| MCTA | 972 | CB PHE A 124 | | | | 62.874 | 1.00 31.20 | 6 |
| | 973 | CG PHE A 124 | | 35.645 | | | | 6 |
| ATOM | | CD1 PHE A 124 | | 34.679 | 38.139 | 62.564 | | |
| ATOM | 974 | CDI PRE A 124 | | 35.378 | | 62.579 | 1.00 29.53 | 6 |
| ATOM | 975 | CD2 PHE A 124 | | | | | | 6 |
| ATOM | 976 | CE1 PHE A 124 | | 33.463 | | | | 6 |
| | | CE2 PHE A 124 | | 34.165 | 40.813 | | | |
| ATOM | 977 | | | 33.207 | | 61.686 | 1.00 28.72 | 6 |
| ATOM | . 978 | CZ PHE A 124 | | | | | | 6 |
| ATOM | 979 | C PHE A 124 | | 37.880 | | | | 8 |
| ATOM | 980 | O PHE A 124 | | 38.427 | | | | 7 |
| ATOM | | 3 3 3 1 3 5 | | 37.545 | | 60.696 | | |
| ATOM | 981 | N ASN A 125 | | 37.731 | | | 1.00 30.10 | 6 |
| ATCM | 982 | CA ASN A 125 | | | | | | 6 |
| | 983 | CB ASN A 125 | | 38.247 | | | | 6 |
| ATOM | | 00 301 3 125 | | 38.281 | | 57.195 | 1.00 33.79 | 0 |
| ATOM | 984 | CG ASN A 125 | | | | | 1.00 31.85 | 8 |
| ATOM | 985 | OD1 ASN A 125 | | 38.754 | | | | 7 |
| | 986 | ND2 ASN A 125 | | 37.790 | 34.268 | | | 6 |
| ATOM | | | | 36.403 | 37.083 | | | |
| ATOM | 987 | C ASN A 125 | | 35.62 | | | 1.00 27.24 | . 8 |
| ATOM | 988 | O ASN A 125 | | | | | | 7 |
| ATOM | 989 | N PRO A 126 | | 36.13 | | | | 6 |
| CN | 990 | CD PRO A 126 | | 36.99 | 7 39.51 | 58.83 | , , | |
| /~ NI | | | | | | | | |

| ATOM | 991 C | A PRO | A 126 | | | 909 | 38.891 | | 7.844 | 1.00 2 | | 6 6 |
|--------------|--------------|-----------------|----------------------|---|-----|----------------|------------------|--------|------------------|--------------|----------------|--------|
| | | B PRO | A 126 | | - | 139 | 40.407 | | 7.856 | 1.00 2 | | 6 |
| ATOM ATOM | | | A 126 | | | 649 | 40.520 | | 7.775 | 1.00 2 | 7 54 | 6 |
| ATOM | 994 C | | A 126 | | | 651 | 38.339 | | 5.448 | 1.00 2 | 9 66 | 8 |
| ATOM | 995 | | A 126 | | | 532 | 38.402 | | 5.949 | 1.00 2 | | 7 |
| ATOM | 996 N | | A 127 | | | 687 | 37.795 | | 5.820 | 1.00 2 | | 6 |
| ATOM | | | A 127 | | | 548 | 37.244 | | 4.477 3.684 | 1.00 2 | 22.43 | 5 |
| ATOM | | | A 127 | | - | 822 | 37.505 | | 4.480 | 1.00 | | 6 |
| ATOM | 999 0 | | A-127 | | | 225 | 35.744 35.140 | | 3.423 | 1.00 | 29.04 | ě. |
| ATOM | 1000 |) ALA | A 127 | | 35. | 038 | 35.140 | 5 | 5.663 | 1.00 | 26.97 | 7 |
| ATOM | 1001 | 1 GLY | A 128 | | | 166 | 33.724 | | 5.737 | 1.00 | 25.65 | 6 |
| MOTA | | A GLY | A 128 | | | 874 389 | 33.486 | | 5.880 | 1.00 | 26.17 | 6 |
| MOTA | | GLY | A 128 | | | 600 | 34.428 | | 5.804 | 1.00 | 27.39 | 8 |
| MOTA | | | A 128 A 129 | | | 998 | 32.234 | | 6.083 | 1.00 | 23.87 | 7 |
| MOTA | | 4 GLY CA GLY | A 129 | | | 588 | 31.936 | 5 | 6.236 | 1.00 | 25.17 | 5 |
| ATOM | | GLY | A 129 | | 30. | 847 | 31.674 | . 5 | 4.937 | 1.00 | | 6 |
| MOTA | | GLY | A 129 | | | 643 | 31.908 | | 4.848 | | 25.07 | 8 7 |
| MOTA | | N MET | A 130 | | | . 566 | 31.198 | | 3.927 | 1.00 | 25.69 26.48 | 6 |
| ATOM ATOM | - | | A 130 | | | .981 | 30.872 | 5 | 2.622 | 1.00 1.00 | | 6 |
| ATOM | | CB MET | A 130 | | | .103 | 30.907 | | 1.567 | 1.00 | 26.54 | 6 |
| MOTA | | CG MET | A 130 | | | .795 | 32.288 | | 0.613 | | 26.29 | 16 |
| ATOM | | | A 130 | | | .413 | 32.366 31.512 | | 9.062 | 1 00 | 25.85 | 6 |
| ATOM | 1014 | | A 130 | | | .080 | 29.463 | - | 2.768 | | 24.47 | 5 |
| MOTA | | | A 130 | | | .355 .761 | 28.502 | | 2.113 | 1.00 | 17.67 | 8 |
| MOTA | | O MET | A 130 | | | .347 | 29.389 | | 3.636 | 1.00 | 23.28 | 7 |
| MOTA | | N HIS | A 131 A 131 | | | .647 | 28.16 | | 4.019 | 1.00 | 26.33 | 6 |
| MOTA | | CA HIS | A 131 | | | .685 | 28.485 | | 55.180 | | 26.98 | 6 |
| MOTA | | | A 131 | | | .663 | 29.540 | - | 54.862 | | 28.50 | 6 |
| ATOM | | CD2 HIS | A 131 | | 26 | .225 | 30.03 | - | 53.677 | | 28.65 | 6 7 |
| MOTA MOTA | | ND1 HIS | A 131 | | 25 | .906 | 30.16 | | 55.831 | | 33.04 27.75 | 6 |
| ATOM | 1023 | CE1 HIS | S A 131 | | | .051 | 30.99 | | 55.259 | | 26.97 | 7 |
| ATOM | 1024 | NE2 HIS | 5 A 131 | | | .224 | 30.93 | | 53.952 53.017 | | 28.44 | 6 |
| MOTA | 1025 | | 5 A 131 | | | .917 | 27.28 26.21 | | 53.390 | | 31.15 | .3 |
| ATOM | 1026 | O HIS | 5 A 131 | | | .434 | 27.69 | | 51.756 | 1.00 | 30.64 | 7 |
| MOTA | 1027 | N HIS | A 132 | | | .861 | 26.93 | - | 50.746 | 1.00 | 28.71 | 6 |
| ATOM | 1028 | CA HIS | 5 A 132 | | | .321 | 27.94 | | 49.890 | 1.00 | 27.21 | 6 |
| MOTA | 1029 | CB HIS | S A 132 S A 132 | | | .408 | 28.81 | | 50.693 | | 28.83 | 6 |
| ATOM | 1030 1031 | CG HIS | S A 132 | | | .111 | 30.13 | 7 | 50.578 | 1.00 | 28.92 | 6 |
| MOTA | 1031 | ND1 HTS | S A 132 | | | .686 | 28.36 | - | 51.773 | | 31.80 | 7 6 |
| MOTA | 1032 | CE1 HI | S A 132 | | | .981 | 29.35 | | 52.285 | 1.00 | | 7 |
| ATOM ATOM | 1034 | NE2 HI | S A 132 | | | 1.222 | 30.44 | | 51.579 49.851 | 1.00 | | 6 |
| ATOM | 1035 | C HI | S A 132 | | 27 | 7.889 | 25.97 | 0 | 49.831 | | 23.44 | 8 |
| ATOM | 1036 | O HI | s a 132 | | 27 | 7.399 | 24.37 | 20 | 49.455 | | 27.94 | 7 |
| ATOM | 1037 | N AL | A A 133 | | | 0.093 | 26.37 25.38 | | 48.579 | | 26.99 | 6 |
| ATOM | 1038 | | A A 133 | | | 9.958 1.295 | | | 48.392 | 1.00 | 21.87 | 6 |
| MOTA | 1039 | | A A 133 | | | 0.199 | | | 49.078 | 1.00 | 26.69 | 6 |
| MOTA | 1040 | C AL | •• •• | • | | 0.703 | | | 50.182 | | 28.25 | 8 |
| MOTA | 1041 | O AL | A A 133 E A 134 | | | 9.850 | | | 48.255 | 1.00 | 26.73 | 7 |
| MOTA | 1042 | | E A 134 | | | 0.046 | | | 48.615 | | 25.04 | 6 |
| MOTA | 1043 1044 | | E A 134 | | | 9.070 | 20.85 | 55 | 47.875 | | 19.20 | 6 6 |
| MOTA | | | E A 134 | | | 7.629 | 21.19 | 99 | 48.100 | | 15.75 | 6 |
| ATOM | 1045 1046 | CD1 PH | E A 134 | | 2 | 6.929 | 21.9 | | 47.169 | | 14.83 14.03 | 6 |
| MOTA MOTA | 1047 | CD2 PH | E A 134 | | | 6.985 | | | 49.273 | | 14.84 | |
| MOTA | 1048 | CE1 PH | E A 134 | | | 5.614 | | | 47.404 | | 12.07 | |
| ATOM | 1049 | CE2 PH | IE A 134 | | 2 | 5.670 | 21.1 | | 48.58 | | 14.59 | 6 |
| ATOM | 1050 | CZ PH | IE A 134 | | | 4.985 | | | 48.31 | | 29.48 | 6 |
| ATOM | 1051 | C PH | IE A 134 | | | 1.460 | _ | 56 | 47.82 | | 33.19 | 8 |
| ATOM | 1052 | | IE A 134 | | | 2.291 1.713 | | | 48.62 | 0 1.00 | 31.52 | 7 |
| ATOM | 1053 | N LY | (S A 135 | | | 3.012 | | 27 | 48.42 | 7 1.00 | 29.15 | , 6 |
| ATOM | 1054 | | (S A 135 | | | 2.92 | | | 48.88 | 5 1.00 | 0 29.45 | |
| ATCM | 1055 | | (S A 135 (S A 135 | | 3 | 4.15 | | 31 | 48.63 | | 0 32.46 | , 6 |
| NOM: | 1056 | CG L' | CCT M CI | | ر | | - - | | - | | | |

| | | CD | LYS A | 135 | 33 | 965 | 15.734 | 49.221 | 1.00 29.67 | 6 |
|--------|-------|-----------|-------|---------|-----|-------|--------|--------|--------------|--------|
| MOTA | 1057 | | | | _ | .234 | 15.703 | 50.716 | 1.00 30.09 | 6 |
| ATOM | 1058 | | LYS A | | | 679 | 15.973 | 51.001 | 1.00 26.25 | 7 |
| MOTA | 1059 | | LYS A | | | | 19.516 | 46.993 | 1.00 30.22 | 6 |
| MOTA | 1060 | | LYS A | | | .513 | 19.672 | 46.763 | 1.00 30.00 | 8 |
| ATOM | 1061 | | LYS A | | | .714 | | 46.028 | 1.00 31.69 | 7 |
| ATOM | 1062 | N | SER A | | | .600 | 19.434 | | 1.00 32.88 | 6 |
| ATOM | 1063 | CA | SER A | 136 | 32 | .995 | 19.489 | 44.619 | 1.00 32.88 | 6 |
| ATOM | 1064 | CB | SER A | 136 | 33 | .038 | 18.077 | 44.040 | 1.00 31.41 | 8 |
| ATOM | 1065 | OG | SER A | | 33 | .882 | 17.241 | 44.810 | 1.00 35.41 | |
| ATOM | 1066 | C | SER A | | 32 | . 097 | 20.347 | 43.727 | 1.00 33.55 | 6 |
| | 1067 | Õ | SER A | | | .921 | 20.031 | 42.553 | 1.00 36.11 | 8 |
| ATOM | 1068 | N | ARG A | | 31 | .536 | 21.425 | 44.262 | 1.00 30.61 | 7 |
| MOTA | 1069 | CA | ARG A | | | . 664 | 22.272 | 43.459 | 1.00 32.28 | .6 |
| ATOM | 1070 | CB | ARG A | | 29 | .324 | 21.554 | 43.202 | 1.00 35.91 | 6 |
| ATOM | | CG | ARG A | 137 | | .224 | 22.458 | 42.627 | 1.00 43.90 | 6 |
| MOTA | 1071 | CD | ARG A | | 26 | .819 | 21.836 | 42.751 | 1.00 48.28 | 6 |
| MOTA | 1072 | NE | ARG A | 137 | | .571 | 20.767 | 41.787 | 1.00 53.38 | 7 |
| MOTA | 1073 | | ARG A | | | .150 | 20.960 | 40.538 | 1.00 55.30 | 6 |
| ATOM | 1074 | CZ | ARG A | 137 | | .921 | 22.185 | 40.090 | 1.00 54.06 | 7 |
| MOTA | 1075 | NHI | ARG A | 137 | | .969 | 19.922 | 39.728 | 1.00 58.96 | 7 |
| ATOM | 1076 | | ARG A | 137 | | .405 | 23.631 | 44.113 | 1.00 30.24 | 6 |
| MOTA | 1077 | C | ARG A | 127 | | .380 | 23.748 | 45.338 | 1.00 23.11 | 8 |
| MOTA | 1078 | 0 | ARG A | | | .219 | 24.653 | 43.279 | 1.00 27.33 | 7 |
| ATOM | 1079 | N | ALA A | | | .944 | 26.000 | 43.757 | 1.00 27.36 | 6 |
| ATOM | 1080 | CA | ALA A | 7 138 | | .149 | 26.997 | 42.645 | 1.00 27.57 | 6 |
| MOTA | 1081 | CB | ALA A | | | .496 | 26.003 | 44.213 | 1.00 26.45 | 6 |
| MOTA | 1082 | С | ALA A | | | | 25.083 | 43.865 | 1.00 27.30 | 8 |
| MOTA | 1083 | 0 | ALA A | | | .747 | 27.021 | 44.975 | 1.00 22.47 | 7 |
| ATOM | 1084 | Ŋ | ASN A | | | .090 | | 45.471 | 1.00 23.85 | 6 |
| ATOM | 1085. | CA | ASN A | 1 139 | | .711 | 27.063 | 46.218 | 1.00 16.82 | 6 |
| ATOM | 1086 | CB | | A 139 | | .406 | 25.738 | 46.900 | 1.00 14.45 | 6 |
| ATOM | 1087 | CG | | A 139 | | .040 | 25.718 | 46.319 | 1.00 13.39 | 8 |
| ATOM | 1088 | OD1 | ASN A | A 139 | | .019 | 26.084 | 48.139 | 1.00 20.08 | 7 |
| ATOM | 1089 | ND2 | ASN A | A 139 | | .018 | 25.249 | 46.139 | 1.00 26.09 | 6 |
| ATOM | 1090 | С | ASN A | A 139 · | | .444 | 28.277 | 47.260 | 1.00 27.50 | 8 |
| ATOM | 1091 | 0 | ASN | A 139 | | 1.239 | 28.600 | | 1.00 24.83 | 7 |
| ATOM | 1092 | N | GLY A | A 140 | | .326 | 28.954 | 46.114 | 1.00 22.24 | 6 |
| ATOM | 1093 | CA | | A 140 | | 1.965 | 30.106 | 46.916 | 1.00 22.35 | 6 |
| ATOM | 1094 | С | GLY . | A 140 | | .991 | 31.211 | 46.890 | 1.00 23.50 | 8 |
| ATOM | 1095 | 0 | GLY . | A 140 | | 5.256 | 31.843 | 47.910 | 1.00 25.60 | 7 |
| MOTA | 1096 | N | | A 141 | | 5.570 | 31.437 | 45.717 | 1.00 25.00 | 6 |
| ATOM | 1097 | CA | | A 141 | | 7.582 | 32.476 | 45.518 | 1.00 28.05 | 6 |
| ATOM | 1098 | CB | | A 141 | | 7.204 | 33.765 | 46.258 | | 6 |
| ATOM | 1099 | CG | PHE | A 141 | | 5.925 | 34.391 | 45.792 | | 6 |
| ATOM | 1100 | CD1 | PHE | A 141 | | 5.352 | 35.428 | | | 6 |
| ATOM | 1101 | CD2 | PHE | | 2 : | 5.312 | 33.975 | | | 6 |
| MO A | 1102 | CE1 | PHE | A 141 | 2 | 4.193 | 36.044 | | | 6 |
| A. COM | 1103 | CE2 | PHE | A 141 | 2 | 4.150 | 34.583 | | | 6 |
| ATCM | 1104 | CZ | | A 141 | | 3.589 | 35.621 | | 1.00 32.59 | |
| ATOM | 1105 | Ċ | PHE | A 141 | 2 | 8.954 | 32.038 | | | 6 8 |
| | 1106 | ō | | A 141 | | 9.938 | 32.727 | | | 7 |
| ATOM | 1107 | Ŋ | | A 142 | 2 | 9.025 | 30.897 | | | |
| MOTA | 1108 | CA | | A 142 | 3 | 0.296 | 30.399 | | | 6 |
| MOTA | | C3 | | A 142 | | 0.062 | 29.787 | 48.567 | | 6 |
| MOTA | 1109 | SG | | A 142 | | 8.943 | 30.748 | | 1.00 22.93 | 16 |
| ATOM | 1110 | | CYS | A 142 | | 1.017 | 29.366 | | 1.00 22.13 | . 6 |
| MOTA | 1111 | c | CIS | A 142 | | 0.408 | 28.389 | | 1.00 22.97 | . 8 |
| ATOM | 1112 | 0 | TVD | A 143 | | 2.317 | 29.573 | | 1.00 23.09 | 7 |
| ATOM | 1113 | <i>N</i> | TIK | A 143 | | 3.129 | 28.632 | | 1.00 23.05 | 6 |
| MOTA | 1114 | CA | | | 3 | 4.063 | | | 1.00 21.60 | |
| MOTA | 1115 | CB | TYK | A 143 | | 3.377 | | | 1.00 24.09 | |
| ATOM | 1116 | CG | YK | A 143 | | 2.969 | | | 1.00 23.29 | 6 |
| ATOM | 1117 | | | A 143 | | 2.365 | | | 1.00 23.26 | , 6 |
| ATOM | 1118 | CE: | TYR | A 143 | | 3.154 | | | | . 6 |
| ATOM | 1119 | ČD: | | A 143 | د . | 2.544 | | | 7 1.00 24.82 | 6 |
| ATOM | 1120 | CE: | | A 143 | 5 | 2.153 | | | | , 6 |
| ATOM | 1121 | CZ | TYR | A 143 | | | | | | |
| ATOM | 1122 | OH | TYR | A 143 | 3 | 1.553 | 33.24. | | | |
| | | | | • | | | | | | |

| | | | 22.000 | 27.766 | 46.290 | 1.00 24.22 | 6 |
|-------|------|---------------|----------|---------|--------|------------|--------|
| MOTA | 1123 | C TYR A 143 | 33.960 | | 45.998 | 1.00 24.58 | 8 |
| ATOM | 1124 | O TYR A 143 | 34.266 | 26.606 | | 1.00 23.83 | 7 |
| ATOM. | 1125 | N ILE A 144 | 34.327 | 28.329 | 47.437 | | |
| | 1126 | CA ILE A 144 | 35.086 | 27.566 | 48.425 | 1.00 20.24 | 6 |
| ATOM | | | 36.547 | 27.982 | 48.453 | 1.00 17.27 | 6 |
| MOTA | 1127 | | 37.231 | 27.354 | 49.662 | 1.00 11.03 | 6 |
| MOTA | 1128 | CG2 ILE A 144 | | 27.603 | 47.110 | 1.00 14.93 | 6 |
| ATCM | 1129 | CG1_ILE A 144 | 37.185 | | 46.946 | 1.00 19.68 | 6 |
| ATOM | 1130 | CD1 ILE A 144 | 38.601 | 28.028 | | 1.00 21.77 | 6 |
| MOTA | 1131 | C ILE A 144 | 34.495 | 27.703 | 49.815 | | 8 |
| | 1132 | O ILE A 144 | 34.288 | 28.811 | 50.318 | 1.00 21.19 | |
| ATOM | 1133 | N ASN A 145 | . 34,212 | 26.555 | 50.424 | 1.00 23.00 | 7 |
| MOTA | | | 33.616 | 26.508 | 51.750 | 1.00 20.92 | 6 |
| ATOM | 1134 | | 32.902 | 25.170 | 51.935 | 1.00 17.08 | 6 |
| MOTA | 1135 | CB ASN A 145 | 32.079 | 25.125 | 53.203 | 1.00 21.04 | 6 |
| MOTA | 1136 | CG ASN A 145 | | | 54.276 | 1.00 20.97 | 8 |
| ATOM | 1137 | OD1 ASN A 145 | 32.549 | 25.508 | 53.093 | 1.00 20.93 | 7 |
| ATOM | 1138 | ND2 ASN A 145 | 30.844 | 24.640 | | 1.00 19.68 | 6 |
| ATOM | 1139 | C ASN A 145 | 34.706 | 26.669 | 52.806 | | 8 |
| ATOM | 1140 | O ASN A 145 | 35.201 | 25.679 | 53.351 | 1.00 20.64 | |
| | 1141 | N ASN A 146 | 35.079 | 27.911 | 53.100 | 1.00 16.28 | 7 |
| MOTA | | CA ASN A 146 | 36.123 | 28.143 | 54.088 | 1.00 19.34 | 6 |
| MOTA | 1142 | | 36.428 | 29.651 | 54.207 | 1.00 20.27 | 6 |
| MOTA | 1143 | | 35.292 | 30.444 | 54.795 | 1.00 18.05 | 6 |
| MOTA | 1144 | CG ASN A 146 | | 30.421 | 55.999 | 1.00 25.83 | 8 |
| MOTA | 1145 | OD1 ASN A 146 | 35.079 | 31.149 | 53.948 | 1.00 16.04 | 7 |
| ATOM | 1146 | ND2 ASN A 146 | 34.552 | | | 1.00 20.48 | 6 |
| ATOM | 1147 | C ASN A 146 | 35.775 | 27.504 | 55.443 | 1.00 19.88 | 8 |
| MOTA | 1148 | C ASN A 146 | 36.663 | 27.027 | 56.151 | | 7 |
| | 1149 | N PRO A 147 | 34.482 | 27.485 | 55.819 | 1.00 19.38 | |
| ATOM | 1150 | CD PRO A 147 | 33.312 | 28.068 | 55.135 | 1.00 17.48 | 6 |
| MOTA | | CA PRO A 147 | 34.058 | 26.877 | 57.087 | 1.00 22.25 | 6 |
| ATOM | 1151 | | 32.539 | 27.065 | 57.057 | 1.00 20.15 | 6 |
| MOTA | 1152 | | 32.407 | 28.378 | 56.305 | 1.00 20.81 | 6 |
| MOTA | 1153 | CG PRO A 147 | 34.443 | 25.383 | 57.188 | 1.00 26.89 | 6 |
| ATOM | 1154 | C PRO A 147 | | | | 1.00 29.10 | 8 |
| ATOM | 1155 | O PRO A 147 | 35.066 | 24.954. | 56.176 | 1.00 25.88 | 7 |
| ATOM | 1156 | N ALA A 148 | 34.070 | 24.596 | | 1.00 25.47 | 6 |
| MOTA | 1157 | CA ALA A 148 | 34.372 | 23.164 | 56.174 | 1.00 23.47 | 6 |
| ATOM | 1158 | CB ALA A 148 | 33.670 | 22.468 | 55.009 | 1.00 21.84 | |
| | 1159 | C ALA A 148 | 35.870 | 22.916 | 56.100 | 1.00 25.94 | 6 |
| MOTA | 1160 | O ALA A 148 | 36.382 | 21.971 | 56.701 | 1.00 27.19 | 8 |
| MOTA | | | 36.574 | 23.756 | 55.349 | 1.00 26.11 | 7 |
| MOTA | 1161 | | 38.017 | 23.609 | 55.233 | 1.00 24.04 | 6 |
| MOTA | 1162 | | 38.622 | 24.663 | 54.267 | 1.00 26.16 | 6 |
| ATOM | 1163 | CB VAL A 149 | 40.135 | 24.476 | 54.158 | 1.00 25.36 | 6 |
| MOTA | 1164 | CG1 VAL A 149 | | 24.544 | 52.886 | 1.00 26.81 | 6 |
| ATOM | 1165 | CG2 VAL A 149 | 37.970 | | 56.640 | 1.00 23.57 | 6 |
| ATOM | 1166 | C VAL A 149 | 38.516 | 23.870 | | 1.00 19.75 | 8 |
| ATOM | 1167 | O VAL A 149 | 39.453 | 23.228 | 57.122 | | 7 |
| MOTA | 1168 | N GLY A 150 | 37.850 | 24.815 | 57.299 | 1.00 22.20 | |
| | 1169 | CA GLY A 150 | 38.210 | 25.175 | 58.654 | 1.00 25.43 | 6 |
| MOTA | 1170 | C GLY A 150 | 38.130 | 23.975 | 59.568 | 1.00 27.19 | 6 |
| ATOM | | | 39.112 | 23.620 | 60.221 | 1.00 27.05 | 8 |
| MOTA | 1171 | O GLY A 150 | 36.959 | 23.348 | 59.618 | | 7 |
| ATOM | 1172 | N ILE A 151 | 36.775 | 22.176 | 60.457 | | 6 |
| ATOM | 1173 | CA ILE A 151 | | 21.654 | 60.389 | | 6 |
| ATCM | 1174 | CB ILE A 151 | 35.317 | | 60.869 | | 6 |
| ATOM | 1175 | CG2 ILE A 151 | 35.251 | 20.215 | | | 6 |
| ATOM | 1176 | CG1 ILE A 151 | 34.394 | 22.540 | 61.240 | | 6 6 |
| ATOM | 1177 | | 34.255 | 23.967 | 60.759 | | 9 |
| | 1178 | | 37.723 | 21.039 | 60.075 | 1.00 29.32 | 6 |
| ATOM | | | 38.340 | 20.420 | 60.947 | | 8 |
| MOTA | 1179 | | 37.843 | | | 1.00 29.91 | 7 |
| atom | 1180 | | 38.704 | | | 1.00 32.58 | 6 |
| ATOM | 1181 | | 30.704 | | | | 6 |
| ATCM | 1182 | | 38.575 | | | | 6 |
| ATOM | 1183 | CG GLU A 152 | 37.269 | 18.848 | | | 6 |
| ATOM | 1184 | CD GLU A 152 | 37.120 | | | | 8 |
| ATOM | 1185 | | 36.089 | | | | 8 |
| | 1186 | | 38.030 | | | | |
| ATOM | 1187 | | 40.145 | | | | 6 |
| ATOM | | | 40.879 | | | 1.00 30.15 | 8 |
| ATOM | 1188 | 9 O GLU A 152 | | | - | | |

| _ | | | ms.m 3 | 163 | | 40.541 | 21.170 | 58.765 | 1.00 33.90 | 7 |
|--------|------|------------|--------|-----|---|--------|-----------------|----------------|------------|-----|
| ATOM | 1189 | N | TYR A | | | 41.875 | 21.563 | 59.193 | 1.00 32.04 | 6 |
| ATOM | 1190 | CA | TYR A | | | | | 59.058 | 1.00 34.88 | 6 |
| ATOM | 1191 | CB | TYR A | | | 42.019 | 23.074 | | | |
| ATOM | 1192 | CG | TYR A | | | 43.280 | 23.667 | 59.639 | 1.00 38.03 | 6 |
| MCTA | 1193 | CD1 | TYR A | 153 | | 44.498 | 23.611 | 58.948 | 1.00 42.34 | 6 |
| ATOM | 1194 | CE1 | TYR A | 153 | | 45.658 | 24.207 | 59.475 | 1.00 43.38 | 6 |
| ATOM | 1195 | CD2 | TYR A | | | 43.250 | 24.321 | 60.869 | 1.00 37.19 | 6 |
| ATOM ' | 1196 | CE2 | TYR A | | | 44.387 | 24.913 | 61.401 | 1.00 41.09 | 6 |
| | 1197 | CZ | TYR A | | | 45.587 | 24.860 | 60.704 | 1.00 43.34 | 6 |
| MOTA | | | TYR A | | | 46.696 | 25.480 | 61.241 | 1.00 44.86 | 8 |
| ATOM | 1198 | | | | | 41.919 | 21.168 | 60.667 | 1.00 32.59 | 6 |
| ATOM | 1199 | C | TYR A | | | | 20.518 | 61.120 | 1.00 32.24 | 8 |
| ATOM | 1200 | 0 | TYR A | | | 42.867 | | _ | 1.00 32.24 | 7 |
| MCTA | 1201 | N | LEU A | | - | 40.869 | 21.556 | 61.397 | | 6 |
| MOTA | 1202 | CA | LEU A | | | 40.730 | 21.261 | 62.823 | 1.00 29.38 | |
| ATOM | 1203 | CB | LEU A | 154 | | 39.443 | 21.889 | 63.378 | 1.00 28.60 | 6 |
| ATOM | 1204 | CG | LEU A | | | 39.399 | 23.407 | 63.618 | 1.00 31.20 | 6 - |
| ATOM | 1205 | CD1 | LEU A | 154 | | 37.991 | 23.833 | 64.041 | 1.00 28.53 | 6 |
| ATOM | 1206 | | LEU A | | | 40.418 | 23 <i>.</i> 787 | 64.691 | 1.00 24.95 | 6 |
| ATOM | 1207 | C | LEU A | | | 40.732 | 19.772 | 63.146 | 1.00 29.56 | 6 |
| | 1208 | ō | LEU A | | | 41.223 | 19.363 | 64.196 | 1.00 28.36 | 8 |
| ATOM | | Ŋ | ARG A | | | 40.174 | 18.958 | 62.256 | 1.00 31.95 | 7 |
| ATOM | 1209 | | ARG A | | | 40.134 | 17.522 | 62.499 | 1.00 33.00 | 6 |
| ATOM | 1210 | CA | | | | | 16.847 | 61.561 | 1.00 33.13 | 6 |
| ATOM | 1211 | CB | ARG A | | | 39.127 | | 61.769 | 1.00 32.84 | 6 |
| ATOM | 1212 | CG | ARG A | | | 37.708 | 17.368 | | 1.00 32.92 | 6 |
| MOTA | 1213 | CD | ARG A | | | 36.678 | 16.719 | 60.863 | | 7 |
| MOTA | 1214 | ΝE | ARG A | | | 36.152 | 15.451 | 61.363 | 1.00 33.98 | |
| ATOM | 1215 | CZ | ARG A | 155 | | 35.195 | 14.760 | 60.741 | 1.00 37.93 | 6 |
| ATOM | 1216 | NH1 | ARG A | 155 | | 34.671 | 15.216 | 59.605 | 1.00 38.39 | 7 |
| ATOM | 1217 | NH2 | ARG A | 155 | | 34.732 | 13.631 | 61.259 | 1.00 38.67 | 7 |
| ATOM | 1218 | С | ARG A | 155 | | 41.521 | 16.929 | 62.331 | 1.00 33.97 | 6 |
| ATOM | 1219 | ō | ARG A | | • | 41.869 | 15.941 | 62.985 | 1.00 32.95 | 8 |
| | 1220 | N | LYS A | | | 42.318 | 17.548 | 61.467 | 1.00 34.20 | 7 |
| ATOM | | CA | LYS A | | | 43.679 | 17.081 | 61.243 | 1.00 36.32 | 6 |
| MCTA | 1221 | | LYS A | | | 44.249 | 17.662 | 59.942 | 1.00 37.57 | 6 |
| ATCM | 1222 | CB | | | | 45.673 | 17.187 | 59.638 | 1.00 40.32 | 6 |
| ATOM | 1223 | CG | LYS A | | | | 17.532 | 58.220 | 1.00 40.33 | 6 |
| ATOM | 1224 | CD | LYS A | | | 46.116 | | 57.184 | 1.00 41.27 | 6 |
| ATOM | 1225 | CE | LYS A | | | 45.180 | 16.909 | | 1.00 37.92 | 7 |
| ATOM | 1226 | NZ | LYS A | | | 45.015 | 15.435 | 57.364 | | 6 |
| ATOM | 1227 | С | LYS A | 156 | | 44.539 | 17.501 | 62.428 | 1.00 36.17 | |
| ATOM | 1228 | 0 | LYS A | 156 | | 45.582 | 16.905 | 62.699 | 1.00 34.53 | 8 |
| ATOM | 1229 | N | LYS A | 157 | | 44.093 | 18.537 | 63.132 | 1.00 36.71 | 7 |
| ATOM | 1230 | CA | LYS A | 157 | | 44.820 | 19.026 | 64.294 | 1.00 37.09 | 6 |
| ATOM | 1231 | CB | LYS A | | | 44.495 | 20.501 | 64.566 | 1.00 37.02 | 6 |
| ATOM | 1232 | CG | LYS A | | | 44.982 | 21.435 | 63.477 | 1.00 36.22 | 6 |
| | 1233 | CD | LYS A | | | 46.468 | 21.231 | 63.239 | 1.00 37.91 | 6 |
| ATOM | 1234 | Œ | LYS A | | | 46.993 | 22.100 | 62.107 | 1.00 39.35 | 6 |
| ATOM | | | LYS A | | | 48.434 | 21.815 | 61.842 | 1.00 38.78 | 7 |
| ATOM | 1235 | -1Z | | | | 44.498 | 18.178 | 65.515 | 1.00 35.61 | 6 |
| ATOM | 1236 | - , | LYS A | | | | 18.232 | 66.518 | 1.00 36.38 | 8 |
| ATOM | 1237 | 0 | LYS A | | | 45.204 | | | 1.00 34.37 | 7 |
| ATOM | 1238 | N | GLY A | | | 43.433 | 17.392 | 65.431 | 1.00 38.08 | 6 |
| ATOM | 1239 | CA | GLY A | | | 43.097 | 16.537 | 66.552 | | |
| ATOM | 1240 | ·C | GLY A | 158 | | 41.782 | 16.781 | 67.267 | 1.00 38.78 | 6 |
| ATOM | 1241 | 0 | GLY A | 158 | | 41.460 | 16.053 | 68.208 | 1.00 41.07 | 8 |
| ATOM | 1242 | N | PHE A | 159 | | 41.023 | 17.791 | 66.855 | 1.00 36.75 | 7 |
| MCTA | 1243 | CA | PHE A | | | 39.743 | 18.046 | 67.505 | 1.00 33.83 | 6 |
| | 1244 | CB | PHE A | | | 39.246 | 19.459 | 67.213 | 1.00 32.65 | 6 |
| ATOM | 1245 | CG | PHE A | | | 40.115 | 20.521 | 67.78 7 | 1.00 29.97 | 6 |
| ATOM | | | | | | 41.404 | 20.724 | 67.297 | 1.00 30.20 | 6 |
| ATOM | 1246 | | PHE A | | | 39.672 | 21.289 | 68.853 | 1.00 29.28 | 6 |
| MOTA | 1247 | CD2 | PHE A | | | | 21.680 | 67.862 | 1.00 28.96 | 6 |
| ATOM | 1248 | CE1 | PHE A | | | 42.241 | | 69.428 | 1.00 29.67 | 5 |
| ATOM | 1249 | CE2 | PHE A | | | 40.498 | 22.246 | | 1.00 29.67 | - 6 |
| ATOM | 1250 | CZ | PHE A | | | 41.785 | 22.442 | 68.931 | | 6 |
| ATCM | 1251 | С | PHE A | | | 38.732 | 17.026 | 67.025 | 1.00 33.41 | |
| ATOM | 1252 | 0 | PHE A | | | 38.664 | 16.716 | 65.838 | 1.00 31.61 | 8 |
| ATOM | 1253 | N | LYS A | | | 37.951 | 16.506 | 67.966 | 1.00 35.13 | 7 |
| | 1254 | CA | LYS A | | | 36.947 | 15.493 | 67.677 | 1.00 35.39 | 6 |
| ATOM | 7774 | | 212 | | _ | | | - | • | |

| | | 6 5 | LYS A 1 | 60 | 37. | 342 | 14.198 | 68.389 | 1.00 36.43 | 6 |
|------|------|------------|---------|-----|-----|--------------|--------|--------|------------|--------|
| MOTA | 1255 | CB | LYS A 1 | 60 | - | 535 | 13.502 | 67.708 | 1.00 40.67 | 6 |
| ATOM | 1256 | | LYS A 1 | 60 | 30. | 312 | 12.538 | 68.615 | 1.00 44.68 | 6 |
| MOTA | 1257 | | LYS A 1 | | 38 | 425 | 11.536 | 69.345 | 1.00 49.23 | 6 |
| MOTA | 1258 | CE | LYS A I | 60 | | 593 | 12.182 | 70.411 | 1.00 50.63 | 7 |
| MOTA | 1259 | NZ | LYS A 1 | 60 | | 524 | 15.927 | 68.027 | 1.00 35.94 | 6 |
| MOTA | 1260 | C | LYS A 1 | 60 | | 561 | 15.241 | 67.691 | 1.00 35.72 | 8 |
| ATOM | 1261 | | LYS A 1 | 60 | | .399 | 17.058 | 68.718 | 1.00 34.35 | 7 |
| MOTA | 1262 | N | ARG A 1 | 91 | | . 091 | 17.618 | 69.044 | 1.00 34.95 | 6 |
| ATOM | 1263 | CA | ARG A 1 | 61 | | .771 | 17.525 | 70.535 | 1.00 33.94 | 6 |
| ATOM | 1264 | CB | ARG A 1 | 61 | | | 16.132 | 70.992 | 1.00 38.25 | 6 |
| ATOM | 1265 | CG | ARG A 1 | 6.1 | | . 427 | 16.131 | 72.386 | 1.00 41.17 | 6 . |
| MOTA | 1266 | CD | ARG A 1 | | | . 823 | 16.722 | 73.378 | 1.00 47.64 | 7 |
| MOTA | 1267 | ME | ARG A 1 | 61 | | .719 .912 | 16.233 | 73.705 | 1.00 47.92 | 6 |
| MOTA | 1268 | CZ | ARG A 1 | | | .372 | 15.131 | 73.121 | 1.00 47.56 | 7 |
| ATOM | 1269 | NH1 | ARG A 1 | 61 | | | 16.858 | 74.616 | 1.00 46.95 | 7 |
| ATOM | 1270 | | ARG A 1 | 61 | | . 648 | 19.076 | 68.598 | 1.00 34.58 | 6 |
| MOTA | 1271 | С | ARG A 1 | | | .113 | 19.980 | 69.357 | 1.00 33.77 | 8 |
| ATOM | 1272 | 0 | ARG A 1 | .61 | | .468 | 19.280 | 67.341 | 1.00 31.74 | 7 |
| MOTA | 1273 | 14 | ILE A 1 | | | .741 | 20.594 | 66.735 | 1.00 29.83 | 6 |
| ATOM | 1274 | CA | ILE A 1 | | | .735 | 20.542 | 65.362 | 1.00 29.96 | 6 |
| ATOM | 1275 | CB | ILE A 1 | .62 | | .429 | 21.942 | 64.784 | 1.00 30.57 | 6 |
| MOTA | 1276 | CG2 | ILE A 1 | .62 | | .580 | | 65.522 | 1.00 28.81 | 6 |
| ATOM | 1277 | CG1 | ILE A 1 | | | .801 | 19.891 | 64.224 | 1.00 33.05 | 6 |
| ATOM | 1278 | CD1 | ILE A 1 | .62 | | .537 | 19.685 | 66.560 | 1.00 29.66 | 6 |
| ATOM | 1279 | С | ILE A 1 | | | .300 | 21.050 | 66.266 | 1.00 25.24 | 8 |
| ATOM | 1280 | 0 | ILE A 1 | .62 | | .416 | 20.241 | | 1.00 30.00 | 7. |
| ATOM | 1281 | 21 | LEU A 1 | 163 | 32 | .081 | 22.351 | 66.745 | 1.00 30.48 | 6 |
| ATOM | 1282 | CA | LEU A | 63 | | .754 | 22.945 | 66.617 | 1.00 30.48 | 6 |
| ATOM | 1283 | CВ | LEU A | 63 | | .236 | 23.406 | 67.992 | 1.00 32.23 | 6 |
| ATOM | 1284 | ĊG | LEU A 1 | 163 | | .934 | 24.229 | 68.044 | | 6 |
| ATOM | 1285 | | LEU A | | | .804 | 23.494 | 67.326 | 1.00 31.58 | 6 |
| | 1286 | CD2 | | 163 | 28 | .569 | 24.502 | 69.493 | 1.00 25.00 | 6 |
| MOTA | 1287 | C | LEU A | | 30 | .717 | 24.122 | 65.659 | 1.00 29.23 | |
| MOTA | 1288 | õ | LEU A | | 31 | .596 | 24.980 | 65.654 | 1.00 29.72 | 8 7 |
| MOTA | 1289 | N | TYR A | | 29 | .675 | 24.157 | 64.846 | 1.00 29.68 | |
| MOTA | 1290 | CA | TYR A | | 29 | .500 | 25.244 | 63.899 | 1.00 29.89 | 6 |
| MOTA | 1291 | CB | TYR A | 164 | 29 | .512 | 24.688 | 62.470 | 1.00 27.81 | 6 |
| MOTA | 1292 | CG | TYR A | 164 | 29 | .377 | 25.742 | 61.399 | 1.00 27.79 | 6 |
| ATOM | 1292 | CD1 | | | | .390 | 26.670 | 61.168 | 1.00 24.82 | 6 |
| ATOM | 1294 | CEI | | | 30 | .247 | 27.655 | 60.198 | 1.00 24.51 | 6 |
| MOTA | 1295 | CD2 | | | 28 | 3.216 | 25.827 | 60.631 | 1.00 27.61 | 6 |
| MOTA | 1296 | CE2 | | | | 3.065 | 26.808 | 59.662 | 1.00 25.67 | 6 |
| ATOM | 1297 | ÇZ | TYR A | | 29 | 0.078 | 27.718 | 59.451 | 1.00 25.63 | 6 |
| ATOM | 1298 | ЭН | TYR A | | 28 | 3.898 | 28.704 | 58.506 | 1.00 27.10 | 8 |
| MOTA | 1299 | c. | TYR A | 164 | | 3.149 | 25.907 | 64.218 | 1.00 28.38 | 6 |
| MOTA | 1300 | 5 | TYR A | 164 | 2° | 7.119 | 25.225 | 64.277 | 1.00 29.43 | 8 |
| ATOM | 1300 | 71 | ILE A | 165 | 28 | 3.166 | 27.217 | 64.464 | 1.00 24.30 | 7 |
| ATOM | | CA | ILE A | 165 | | 6.941 | 27.969 | 64.754 | 1.00 22.93 | 6 |
| ATOM | 1302 | СВ | ILE A | 165 | | 6.985 | 28.649 | 66.143 | 1.00 22.00 | 6 |
| MOTA | 1303 | CG | | | | 5.765 | | 66.312 | 1.00 16.15 | 6 |
| MOTA | 1304 | CG: | | 165 | | 7.033 | | | 1.00 20.78 | 6 |
| ATOM | 1305 | | | 165 | | 7.185 | | | 1.00 15.49 | 6 |
| MOTA | 1306 | CD: | ILE A | 165 | | 6.784 | | | 1.00 24.45 | 6 |
| ATOM | 1307 | 2 | 155 4 | 165 | | 7.605 | | | 1.00 23.17 | 8 |
| MOTA | 1308 | <u>ي</u> | ILE A | 166 | | 5.709 | | | 1.00 24.20 | 7 |
| MOTA | 1309 | N | ASP A | 166 | | 5.478 | | | 1.00 20.78 | 6 |
| ATOM | 1310 | CA | ASP A | 166 | | 5.314 | _ | | 1.00 17.64 | 6 |
| ATOM | 1311 | 23 | ASP A | 100 | | 5.410 | | | | 6 |
| MOTA | 1312 | CG | ASP A | 100 | | 4.536 | | | 1.00 20.20 | 8 |
| ATOM | 1313 | CD | 1 ASP A | 100 | | | | | | . 8 |
| MOTA | 1314 | | 2 ASP A | 100 | | 6.366 | | | | 6 |
| ATOM | 1315 | | ASP A | 166 | | 4.290 | | | | 8 |
| ATOM | 1316 | 2 | ASP A | 166 | | 3.134 | | | | 7 |
| ATOM | 1317 | | LEU A | 167 | | 4.583 | | | | |
| ATOM | 1318 | | LEU A | 167 | | 3.536 | | | | |
| MOTA | 1319 | | LEU A | 167 | | 3.963 | | | | |
| MOTA | 1320 | | | 167 | 2 | 4.364 | 33.463 | 64.674 | 1.00 20.7. | • |
| MIUN | | | | | | | | | | |

| | | | | | | | | _ |
|-------|-------|----------------|------|--------|--------|---|------------|-----|
| - | | 3 167 | 24 | .741 | 34.647 | 65.552 | 1.00 26.24 | 6 |
| MOTA | 1321 | CD1 LEU A 167 | | | | 65.302 | 1.00 23.45 | 6 |
| MOTA | 1322 | CD2 LEU A 167 | 23 | . 225 | | | 1.00 26.37 | 6 |
| | | C LEU A 167 | 23 | .162 | 33.660 | 60.951 | 1.00 26.37 | |
| MOTA | | | | .386 | 34.613 | 60.971 | 1.00 25.95 | 8 |
| ATOM | 1324 | O LEU A 167 | | | | 59.828 | 1.00 29.66 | 7 |
| ATOM | 1325 | N ASP A 168 | 23 | .726 | 33.208 | | 1.00 28.35 | 6 |
| | | | 23 | .410 | 33.787 | 58.520 | 1.00 28.33 | |
| ATOM- | 1326 | | | .057 | 32.987 | 57.390 | 1.00 33.29 | 6 |
| MOTA | 1327 | CB ASP A 168 | | | | 56.037 | 1.00 35.38 | 6 |
| ATOM | 1328 | CG ASP A 168 | 23 | .937 | 33.676 | | | 8 |
| | | OD1 ASP A -168 | . 24 | .892 | 34.388 | 55.659 | 1.00 39.48 | |
| MOTA | 1329 | ODI ASP A 100 | | .893 | 33.531 | 55.364 | 1.00 33.40 | 8 |
| ATOM | 1330 | OD2 -ASP A 168 | | | | 58.408 | 1.00 28.74 | 6 |
| ATOM | 1331 | C ASP A 168 | 21 | .906 | 33.614 | 55.400 | 1 00 26 21 | 8 |
| | | 160 | 21 | .354 | 32.648 | 58.948 | 1.00 26.21 | |
| ATOM | 1332 | O ASP A 168 | | .239 | 34.524 | 57.711 | 1.00 26.16 | 7 |
| ATOM | 1333 | N ALA A 169 | | | 34.415 | 57.579 | 1.00 24.39 | 6 |
| ATOM | 1334 | CA ALA A 169 | | .793 | | | 1.00 22.75 | 6 |
| | 1335 | CB ALA A 169 | 19 | .233 | 35.640 | 56.879 | 1.00 22.73 | |
| ATOM | | | 19 | .420 | 33.157 | 56.813 | 1.00 24.37 | • |
| ATOM | 1336 | C ALA A 169 | | .266 | 32.752 | 56.824 | 1.00 22.34 | 8 |
| MOTA | 1337 | O ALA A 169 | | | | 56.156 | 1.00 25.78 | 7 |
| ATOM | 1338 | N HIS A 170 | 20 | .405 | 32.542 | 30.130 | 1.00 25.20 | 6 |
| | | CA HIS A 170 | 20 | 180 | 31.327 | 55.375 | | |
| MOTA | 1339 | CA 115 A 170 | | .667 | 31.501 | 53.936 | 1.00 25.76 | 6 |
| MOTA | 1340 | CB HIS A 170 | | | 32.711 | 53.245 | 1.00 29.08 | 6 |
| ATOM | 1341 | CG HIS A 170 | |).122 | | | 1.00 30.59 | 6 |
| | 1342 | CD2 HIS A 170 | 19 | 3.338 | 32.834 | 52.147 | | 7 |
| ATOM | | ND1 HIS A 170 | 2.0 | 384 | 33.995 | 53.675 | 1.00 30.77 | |
| ATOM | 1343 | NOT HIS A 170 | | 784 | 34.858 | 52.873 | 1.00 29.07 | 6 |
| MOTA | 1344 | CE1 HIS A 170 | | | | 51.939 | 1.00 32.19 | 7 |
| ATOM | 1345 | NE2 HIS A 170 | | 9.143 | 34.180 | | 1.00 26.00 | 6 |
| | 1346 | C HIS A 170 | 20 | 0.895 | 30.113 | 55,958 | 1.00 20.00 | |
| ATOM | | | | 1.913 | 30.234 | 56.637 | 1.00 25.76 | 8 |
| ATOM | 1347 | O HIS A 170 | | | 28.939 | 55.658 | 1.00 27.29 | 7 |
| MOTA | 1348 | N HIS A 171 | | 0.349 | | 56.090 | 1.00 25.01 | 6 |
| MOTA | 1349 | CA HIS A 171 | | 0.893 | 27.655 | | 1.00 24.93 | 6 |
| | 1350 | CB HIS A 171 | 19 | 9.934 | 26.532 | 55.663 | 1.00 24.93 | |
| ATOM | | | . 20 | 0.468 | 25.148 | 55.889 | 1.00 26.56 | 6 |
| ATOM | 1351 | CG HIS A 1/1 | | 0.674 | 24.123 | 55.028 | 1.00 22.34 | 6 |
| MOTA | 1352 | CD2 HIS A 171 | | | | 57.137 | 1.00 25.35 | 7 |
| ATOM | 1353 | ND1 HIS A 171 | | 0.823 | 24.678 | | 1.00 22.68 | 6 |
| | 1354 | CE1 HIS A 171 | . 2: | 1.222 | 23.424 | 57.036 | | 7 |
| MOTA | | NE2 HIS A 171 | | 1.140 | 23.062 | 55.767 | 1.00 24.13 | |
| MOTA | 1355 | NEZ 113 A 171 | | 2.267 | 27.413 | 55.471 | 1.00 24.74 | 6 |
| ATOM | 1356 | C HIS A 171 | 2. | 2.20, | 27.863 | 54.356 | 1.00 28.22 | 8 |
| ATOM | 1357 | O HIS A 171 | | 2.540 | | | 1.00 23.03 | 7 |
| | 13'58 | N CYS A 172 | | 3.131 | 26.705 | 56.190 | 1.00 23.41 | 6 |
| ATOM | 1359 | CA CYS A 172 | 2 | 4.467 | 26.389 | 55.683 | | |
| ATOM | | 4 4 7 4 | | 5.497 | 26.474 | 56.812 | 1.00 19.31 | 6 |
| ATOM | 1360 | CB CYS A 1/2 | | 5.005 | 25.631 | 58.318 | 1.00 16.78 | 16 |
| ATOM | 1361 | SG CYS A 172 | | | | 55.048 | 1.00 25.45 | 6 |
| ATOM | 1362 | C CYS A 172 | | 4.484 | 24.997 | | 1.00 24.47 | 8 |
| | 1363 | O CYS A 172 | 2 | 5.203 | 24.098 | 55.483 | 1.00 24.47 | 7 |
| MOTA | | | 2 | 3.664 | 24.839 | 54.015 | 1.00 26.67 | |
| MOTA | 1364 | N ASP A 1/3 | | 3.542 | 23.593 | 53.269 | 1.00 26.47 | 6 |
| ATOM | 1365 | CA ASP A 173 | | | 23.857 | 51.993 | 1.00 26.33 | 6 |
| ATOM | 1366 | CB ASP A 173 | | 2.735 | | 51.555 | 1.00 27.06 | 6 |
| | 1367 | CG ASP A 1 3 | 2 | 3.281 | 25.030 | 51.179 | 1.00 27.00 | |
| MOTA | | OD1 ASP A 173 | 2 | 2.539 | 25.558 | 50.330 | 1.00 23.43 | 8 |
| MOTA | 1368 | ODI MSF A 173 | | 4.454 | 25.417 | 51.372 | 1.00 29.38 | 8 |
| ATOM | 1369 | OD2 ASP A 173 | | | | 52.922 | 1.00 26.65 | 6 |
| MOTA | 1370 | C ASP A 173 | | 4.872 | 22.932 | 50.704 | | 8 |
| | 1371 | O ASP A 173 | 2 | 4.940 | 21.708 | 52.784 | 1.00 20.30 | 7 |
| MOTA | | | 2 | 5.926 | 23.737 | 52.793 | 1.00 25.24 | |
| ATOM | 1372 | N GLY A 174 | | 7.227 | | 52.447 | 1.00 23.11 | 6 |
| MOTA | 1373 | CA GLY A 174 | | | | | | 6 |
| ATOM | 1374 | C GLY A 174 | 2 | 27.896 | 22.505 | | | 8 |
| | | O GLY A 174 | 2 | 28.443 | 21.408 | 53.462 | | 7 |
| MOTA | 1375 | 3 331 3 17E | | 7.848 | | | 1.00 24.29 | , |
| ATCM | 1376 | N VAL A 175 | | | | | | 6 |
| MOTA | 1377 | CA VAL A 175 | 4 | 28.459 | | | | 6 |
| | 1378 | CB VAL A 175 | 7 | 28.536 | 23.672 | | | 6 |
| ATOM | | CG1 VAL A 175 | | 29.449 | | 58.218 | | 2 |
| MOTA | 1379 | | | 29.015 | | 56.530 | 1.00 18.74 | 6 |
| MOTA | 1380 | CG2 VAL A 175 | | | | | 1.00 22.85 | 6 |
| ATCM | 1381 | C VAL A 175 | | 27.647 | | | | 8 |
| | 1382 | | | 28.173 | | | | 7 |
| ATOM | | | : | 26.356 | 21.404 | 56.203 | | 6 |
| ATOM | 1383 | | | 25.518 | | 56.629 | 1.00 27.18 | |
| ATOM | 1384 | | | | | | | . 6 |
| ATOM | 1385 | CB GLN A 176 | | 24.045 | 20.01 | | | |
| 2TOM | 1386 | | | 23.084 | 19.483 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | , | |

| > mow | 1387 | CD GLN A 176 | 21.620 | | | 1.00 38.36 | 6 |
|--------------|--------------|--------------------------------|------------------|------------------|------------------|--------------------------|---------------|
| MOTA MOTA | | OE1 GLN A 176 | 21.113 | | | 1.00 38.59 1.00 38.81 | 8 7 |
| ATOM | | NE2 GLN A 176 | 20.934 | | | 1.00 38.81 | 6 |
| ATOM | | C GLN A 176 | 25.956 | | 55.841 56.416 | 1.00 26.89 | 8 |
| ATOM | 1391 | O GLN A 176 | 26.326 | 18.066 | 54.519 | 1.00 27.96 | 7 |
| ATOM | 1392 | N GLU A 177 | 25.951 | 19.194 18.062 | 53.698 | 1.00 31.16 | 6 |
| MOTA | 1393 | CA GLU A 177 | 26.343 | 18.460 | 52.220 | 1.00 30.37 | 6 |
| MOTA | 1394 | CB GLU A 177 | 26.395 26.353 | 17.256 | 51.287 | 1.00 36.20 | 6 |
| MOTA | 1395 | CG GLU A 177 | 26.273 | 17.626 | 49.818 | 1.00 40.70 | 6 |
| ATOM | 1396 | CD GLU A 177 | 27.322 | 17.967 | 49.234 | 1.00 46.78 | 8 |
| MOTA | 1397 | OE1 GLU A 177 OE2 GLU A 177 | 25.155 | 17.590 | 49.250 | 1.00 39.39 | 8 |
| ATOM | 1398 | | 27.702 | 17.516 | 54.137 | 1.00 31.66 | 6 |
| ATOM | 1399 | O GLU A 177 | 27.868 | 16.317 | 54.356 | 1.00 32.81 | 8 |
| ATOM | 1400 1401 | N ALA A 178 | | 18.419 | 54.287 | 1.00 33.39 | 7 |
| MOTA | 1401 | CA ALA A 178 | 30.026 | 18.072 | 54.673 | 1.00 31.63 | 6 |
| MOTA MOTA | 1403 | CB ALA A 178 | 30.830 | 19.338 | 54.856 | 1.00 30.96 | 6 6 |
| ATOM | 1404 | C ALA A 178 | 30.204 | 17.185 | 55.897 | 1.00 30.63 1.00 27.95 | 8 |
| ATOM | 1405 | O ALA A 178 | 31.032 | 16.276 | 55.876 | 1.00 27.93 | 7 |
| ATOM | 1406 | N PHE A 179 | 29.444 | 17.444 | 56.961 58.184 | 1.00 31.34 | 6 |
| ATOM | 1407 | CA PHE A 179 | 29.590 | 16.656 | 59.310 | 1.00 30.13 | 6 |
| ATOM | 1408 | CB PHE A 179 | 30.147 | 17.532 18.505 | 58.858 | 1.00 27.78 | 6 |
| ATOM | 1409 | CG PHE A 179 | 31.189 30.827 | 19.790 | 58.466 | 1.00 28.24 | 6 |
| MOTA | 1410 | CD1 PHE A 179 | 32.522 | 18.124 | 58.766 | 1.00 28.33 | 6 |
| MOTA | 1411 | CD2 PHE A 179 CE1 PHE A 179 | 31.778 | 20.688 | 57.988 | 1.00 26.68 | 6 |
| MOTA | 1412 | CE1 PHE A 179 CE2 PHE A 179 | 33.487 | 19.013 | 58.285 | 1.00 28.79 | 6 |
| MOTA | 1413 | CZ PHE A 179 | 33.111 | 20.300 | 57.895 | 1.00 28.67 | 6 |
| MOTA | 1414 1415 | C PHE A 179 | 28.300 | 16.003 | 58.664 | 1.00 32.06 | 6 |
| MOTA MOTA | 1416 | O PHE A 179 | 28.218 | 15.542 | 59.803 | 1.00 30.58 | 8 7 |
| ATOM | 1417 | N TYR A 180 | 27.305 | 15.960 | 57.787 | 1.00 34.25 1.00 38.60 | 6 |
| MOTA | 1418 | CA TYR A 180 | 26.001 | 15.377 | 58.099 | 1.00 38.99 | 6 |
| MOTA | 1419 | CB TYR A 180 | 25.062 | 15.605 | 56.911 57.220 | 1.00 37.91 | 6 |
| ATOM | 1420 | CG TYR A 180 · | 23.593 | 15:453 | 57.064 | 1.00 35.83 | 6 |
| MOTA | 1421 | CD1 TYR A 180 | 22.938 | 14.232 14.103 | 57.373 | 1.00 39.20 | 6 |
| ATOM | 1422 | CEL TYR A 180 | 21.589 22.861 | 16 543 | 57.694 | 1.00 37.56 | 6 |
| MOTA | 1423 | CD2 TYR A 180 | 21.518 | 16.430 | 58.007 | 1.00 40.28 | 6 |
| MOTA | 1424 | CE2 TYR A 180 CZ TYR A 180 | 20.882 | 15.211 | 57.848 | 1.00 41.92 | 6 |
| ATOM | 1425 1426 | CZ TYR A 180 OH TYR A 180 | 19.549 | 15.110 | 58.188 | 1.00 43.41 | 8 |
| ATOM | 1427 | C TYR A 180 | 26.133 | 13.884 | 58.382 | 1.00 40.28 | 6 |
| ATOM ATOM | 1428 | O TYR A 180 | 25.158 | 13.192 | 58.680 | 1.00 39.27 | 8 7 |
| ATOM | 1429 | N ASP A 181 | 27.363 | 13.402 | 58.319 | 1.00 43.51 1.00 45.89 | 6 |
| ATOM | 1430 | CA ASP A 181 | 27.638 | 11.994 | 58.519 | 1.00 43.09 | 6 |
| ATOM | 1431 | CB ASP A 181 | 28.414 | 11.487 | 57.303 57.436 | 1.00 56.84 | 6 |
| ATOM | 1432 | CG ASP A 181 | 28.830 | 10.050 | 58.345 | 1.00 59.47 | 8 |
| ATOM | 1433 | OD1 ASP A 181 | 29.637 | 9.750 9.221 | 56.629 | 1.00 60.73 | 8 |
| ATOM | 1434 | OD2 ASP A 181 | 28.348 28.398 | 11.665 | 59.804 | 1.00 44.75 | 6 |
| ATOM | 1435 | C ASP A 181 | 28.257 | 10.568 | 60.350 | 1.00 44.69 | 8 |
| ATOM | 1436 | O ASP A 181 N THR A 182 | 29.194 | 12.606 | 60.298 | 1.00 41.26 | 7 |
| ATOM | 1437 | OA THR A 182 | 29.975 | 12.337 | 61.495 | 1.00 39.51 | 6 |
| ATOM | 1438 1439 | CB THR A 182 | 31.408 | 12.881 | 61.355 | | 6 |
| ATOM | 1440 | OG1 THR A 182 | 32.171 | 12.508 | 62.505 | | 8 6 |
| MOTA MOTA | 1441 | CG2 THR A 182 | 31.395 | | 61.232 | 1.00 40.12 1.00 38.58 | 6 |
| MOTA | 1442 | C THR A 182 | 29.370 | | | | 8 |
| ATOM | 1443 | O THR A 182 | 28.609 | | | | 7 |
| ATOM | 1444 | N ASP A 183 | 29.712 | | | - 44 34 44 | 6 |
| ATOM | 1445 | CA ASP A 183 | 29.211 | | | | 6 |
| ATOM | 1446 | CB ASP A 183 | 28.824 | 11.588 10.723 | | | 6 |
| ATOM | 1447 | CG ASP A 183 | 30.010 | | | | 8 |
| ATOM | 1448 | OD1 ASP A 183 | 30.725 30.221 | | | 1.00 42.46 | 8 |
| MOTA | 1449 | OD2 ASP A 183 | 30.286 | | | 1.00 40.34 | 6 |
| ATOM | 1450 | C ASP A 183 O ASP A 183 | 30.109 | | | 1.00 42.07 | 8 |
| ATOM | 1451 1452 | | 31.400 | | | 1.00 39.29 | 7 |
| TO TO M | 1434 | 14 0000 20 20 2 | | | - | • | |

| | | CA GLN A | 104 | 32.506 | 14.635 | 65.671 | 1.00 37.08 | 6 |
|-------|------|-----------|-------|---------|---------|--------|------------|---|
| ATOM | 1453 | | | 33.830 | 14.252 | 64.994 | 1.00 33.77 | 6 |
| ATOM | 1454 | CB GLN A | | | 12.804 | 65.166 | 1.00 33.63 | 6 |
| MOTA | 1455 | CG GLN A | | 34.229 | | 64.593 | 1.00 32.74 | 6 |
| MOTA | 1456 | CD GLN A | | 35.599 | 12.499 | | 1.00 31.17 | 8 |
| MOTA | 1457 | OE1 GLN A | | 35.853 | 12.704 | 63.413 | | 7 |
| MOTA | 1458 | NE2 GLN A | 184 | 36.490 | 11.999 | 65.436 | 1.00 36.58 | |
| ATOM | 1459 | C GLN A | | 32.222 | 16.110 | 65.403 | 1.00 36.42 | 6 |
| | 1460 | O GLN A | | 32.803 | 16.994 | 66.034 | 1.00 37.41 | 8 |
| MOTA | | N VAL A | | 31.329 | 16.372 | 64.456 | 1.00 33.14 | 7 |
| MOTA | 1461 | | | 30.984 | 17.740 | 64.119 | 1.00 32.40 | 6 |
| ATOM | 1462 | | | 31.308 | 18.052 | 62.641 | 1.00 33.03 | 6 |
| ATOM | 1463 | | | 31.009 | 19.520 | 62.331 | 1.00 29.27 | 6 |
| MOTA. | 1464 | CG1 VAL A | | 32.773 | 17.738 | 62.357 | 1.00 34.58 | 6 |
| ATOM | 1465 | CG2 VAL A | | | 17.730 | 64.360 | 1.00 31.51 | 6 |
| ATOM | 1466 | C VAL A | | 29.508 | 17.124 | 64.038 | 1.00 31.71 | 8 |
| MOTA | 1467 | O VAL A | | 28.680 | | 64.946 | 1.00 30.98 | 7 |
| ATOM | 1468 | N PHE A | 186 | 29.185 | 19.119 | | 1.00 31.44 | 6 |
| ATOM | 1469 | CA PHE A | 186 | 27.798. | | 65.207 | 1.00 30.96 | 6 |
| ATOM | 1470 | CB PHE A | 186 | 27.524 | 19.532 | 66.716 | | 6 |
| ATOM | 1471 | CG PHE A | 186 | 26.059 | 19.617 | 67.066 | 1.00 31.59 | |
| | 1472 | CD1 PHE A | | 25.552 | 18.901 | 68.153 | 1.00 30.54 | 6 |
| MOTA | 1473 | CD2 PHE A | 186 | 25.179 | 20.395 | 66.308 | 1.00 31.50 | 6 |
| MOTA | | CE1 PHE A | 186 | 24.191 | 18.951 | 68.478 | 1.00 33.28 | б |
| MOTA | 1474 | CE2 PHE A | | 23.815 | 20.457 | 66.622 | 1.00 33.04 | 6 |
| MOTA | 1475 | | 106 | 23.318 | 19.733 | 67.708 | 1.00 32.35 | 6 |
| MOTA | 1476 | | | 27.490 | 20.798 | 64.551 | 1.00 30.37 | 6 |
| MOTA | 1477 | C PHE A | 186 | 28.189 | 21.789 | 64.751 | 1.00 31.32 | 8 |
| ATOM | 1478 | O PHE A | 186 | 26.435 | 20.809 | 63.752 | 1.00 31.14 | 7 |
| ATOM | 1479 | N VAL A | | | | 63.063 | 1.00 32.05 | 6 |
| ATOM | 1480 | CA VAL A | | 26.024 | 22.015 | 61.525 | 1.00 33.54 | 6 |
| ATOM | 1481 | CB VAL A | | 26.018 | 21.805 | 60.813 | 1.00 32.07 | 6 |
| ATOM | 1482 | CG1 VAL A | 187 | 25.574 | 23.081 | | 1.00 35.44 | 6 |
| ATOM | 1483 | CG2 VAL A | 187 | 27.420 | 21.389 | 61.056 | 1.00 33.44 | 6 |
| ATOM | 1484 | C VAL A | 187 | 24.638 | 22.439 | 63.524 | 1.00 31.47 | 8 |
| ATOM | 1485 | O VAL A | 187 | 23.666 | 21.686. | 63.410 | 1.00 29.06 | |
| | 1486 | N LEU A | | 24.579 | 23.638 | 64.090 | 1.00 29.44 | 7 |
| MOTA | 1487 | CA LEU A | | 23.336 | 24.228 | 64.551 | 1.00 29.39 | 6 |
| MOTA | 1488 | CB LEU A | | 23.433 | 24.665 | 66.009 | 1.00 29.62 | 6 |
| MOTA | 1489 | CG LEU A | | 22.293 | 25.589 | 66.458 | 1.00 27.92 | 6 |
| MOTA | | CD1 LEU A | | 20.970 | 24.844 | 66.414 | 1.00 25.87 | 6 |
| MOTA | 1490 | CD2 LEU A | 188 | 22.574 | 26,107 | 67.861 | 1.00 27.69 | 6 |
| MOTA | 1491 | | 100 | 23.161 | 25.454 | 63.675 | 1.00 31.89 | 6 |
| ATOM | 1492 | | | 24.130 | 26.175 | 63.388 | 1.00 31.50 | 8 |
| MOTA | 1493 | O LEU A | 100 | 21.929 | 25.700 | 63.250 | 1.00 29.93 | 7 |
| MOTA | 1494 | N SER A | 109 | 21.682 | 26.831 | 62.390 | 1.00 24.65 | 6 |
| MOTA | 1495 | CA SER A | | | 26.411 | 60.942 | 1.00 22.40 | 6 |
| MOTA | 1496 | CB SER A | 189 | 21.873 | 27.485 | 60.083 | 1.00 19.12 | 8 |
| ATOM | 1497 | OG SER A | | 21.585 | | | | 6 |
| ATOM | 1498 | C SER A | | 2016 | 27.462 | 62.577 | 1.00 26.72 | 8 |
| ATOM | 1499 | O SER A | . 189 | 1996 | 26.774 | | 1.00 27.41 | 7 |
| ATOM | 1500 | N LEU A | | 20.121 | 28.783 | 62.669 | 1.00 27.41 | 6 |
| ATOM | 1501 | CA LEU A | 190 | 19.096 | 29.554 | 62.735 | 1.00 29.00 | 6 |
| ATOM | 1502 | CB LEU A | 190 | 19.185 | 30.682 | 63.771 | 1.00 29.84 | |
| | 1503 | CG LEU A | | 19.108 | 30.366 | 65.264 | 1.00 26.79 | 6 |
| ATOM | 1504 | CD1 LEU A | | 19.020 | 31.662 | 66.045 | 1.00 23.44 | 6 |
| ATOM | | CD2 LEU A | 190 | 17.881 | 29.549 | 65.546 | 1.00 27.63 | 6 |
| MOTA | 1505 | | | 19.046 | 30.141 | 61.329 | 1.00 29.58 | 6 |
| MOTA | 1506 | _ | | 20.084 | 30.525 | 60.790 | 1.00 32.40 | 8 |
| MOTA | 1507 | | | 17.864 | | 60.727 | 1.00 29.61 | 7 |
| ATOM | 1508 | N HIS A | | 17.004 | | 59.368 | 1.00 29.72 | 6 |
| MOTA | 1509 | CA HIS A | 7 191 | 17.766 | | 58.432 | | 6 |
| MOTA | 1510 | CB HIS A | 191 | 18.595 | 29.839 | 58.504 | | 6 |
| ATOM | 1511 | CG HIS A | | 18.225 | | | | 6 |
| ATOM | 1512 | CD2 HIS A | 191 | 18.918 | | 58.940 | | 7 |
| | 1513 | ND1 HIS A | 191 | 16.989 | | 58.118 | | 6 |
| ATOM | 1514 | CE1 HIS A | 191 | 16.938 | | | | 7 |
| ATOM | 1515 | NE2 HIS A | 191 | 18.095 | 26.220 | 58.810 | | é |
| ATOM | | C HIS A | 191 | 16.329 | 30.812 | 58.856 | | 6 |
| ATOM | 1516 | | 191 | 15.385 | 30.411 | | 1.00 27.81 | 8 |
| ATOM | 1517 | | 192 | 16.183 | | | | 7 |
| LTCM | 1518 | N GLN 3 | 3 226 | | | • | • | |

| | | | | _ | | | | 22 404 | 57.008 | 1.00 2 | 8.21 | 6 |
|--------|-------|------|--------|-------|---|-----|--------|--------|--------|--------|-------|---|
| ATOM | 1519 | CA (| GLN A | 192 | , | | | 31.494 | 55.796 | 1.00 2 | | 6 |
| ATOM | 1520 | CB (| GLN A | 192 | | | | 32.416 | | 1.00 2 | | 6 |
| MOTA | 1521 | CG · | GLN A | 192 | | 15. | | 33.773 | 56.124 | 1.00 2 | 2.00 | 6 |
| | 1522 | | GLN A | | | 15. | .701 | 34.690 | 54.921 | 1.00 2 | 2.22 | |
| ATOM | | OE1 | GLN A | 192 | | | . 684 | 35.173 | 54.428 | 1.00 2 | | 8 |
| MOTA | 1523 | | GLN A | | | | .914 | 34.925 | 54.434 | 1.00 2 | | 7 |
| ATOM | | NE2 | GLIN A | 100 | | | . 435 | 30.104 | 56.570 | 1.00 3 | 2.71 | 6 |
| ATOM | 1525 | C. | GLN A | 192 | | | | 29.403 | 55.853 | 1.00 3 | 3.85 | 8 |
| MOTA | 1526 | 0 | GLN A | 192 | | | .157 | 29.403 | 57.011 | 1.00 3 | | 7 |
| ATOM | 1527 | N | SER A | 193 | | | .249 | 29.694 | 56.650 | 1.00 3 | | 6 |
| MOTA | 1528 | CA | SER A | 193 | | | .751 | 28.376 | | 1.00 3 | | 6 |
| ATOM | 1529 | CB | SER A | 193 | | | .264 | 28.249 | 56.961 | | | 8 |
| | 1530 | OG | SER A | | | | .786 | 26.987 | 56.540 | 1.00 3 | 1.32 | 6 |
| MOTA | 1531 | c | SER A | 193 | | 12 | .974 | 28.150 | 55.171 | | 34.79 | |
| ATOM | | Ö | SER A | 193 | | 12 | .775 | 29.051 | 54.356 | 1.00 3 | | 8 |
| MOTA | .1532 | | PRO A | 194 | | | .404 | 26.938 | 54.803 | 1.00 3 | | 7 |
| MOTA | 1533 | И | PRO A | | | | .689 | 25.775 | 55.658 | 1.00 | 38.89 | 6 |
| MOTA | 1534 | CD | PRO A | | | | .654 | 26.600 | 53.403 | 1.00 | 37.81 | 6 |
| ATOM | 1535 | CA | PRO A | 104 | | | .248 | 25.194 | 53.498 | 1.00 | 39.30 | 6 |
| ATOM | 1536 | CB | PRO A | 194 | | | .840 | 25.163 | 54.916 | 1.00 | 39.09 | 6 |
| ATOM | 1537 | CG | PRO A | | | | | 26.617 | 52.638 | 1.00 | | 6 |
| MOTA | 1538 | С | PRO A | | | | .340 | | 51.425 | 1.00 | | 8 |
| ATOM | 1539 | 0 | PRO A | | | | .317 | 26.443 | 53.364 | | 39.25 | 7 |
| MOTA | 1540 | N | GLÚ A | 195 | | | .246 | 26.835 | | | 41.54 | 6 |
| ATOM | 1541 | CA | GLU A | 195 | | | .928 | 26.866 | 52.750 | 1.00 | | 6 |
| | 1542 | CB | GLU A | 195 | | | .843 | 26.600 | 53.812 | | | 6 |
| MOTA | 1543 | CG | GLU A | 195 | | 8 | .360 | 27.811 | 54.608 | 1.00 | | |
| MOTA | | CD | GLU A | 195 | | 7 | .160 | 28.502 | 53.960 | 1.00 | 55.91 | 6 |
| ATOM · | | OE1 | GLU A | 195 | | 6 | .735 | 29.571 | 54.461 | 1.00 | | 8 |
| MOTA | 1545 | OEI | GLU A | 195 | | | .631 | 27.966 | 52.956 | 1.00 | | 8 |
| MOTA | 1546 | | GLU A | 105 | | | .700 | 28.208 | 52.047 | | 39.50 | 6 |
| MOTA | 1547 | C | GLU A | | | | 3.651 | 28.431 | 51.452 | | 40.21 | 8 |
| MOTA | 1548 | 0 | | | | | 0.689 | 29.096 | 52.098 | | 37.13 | 7 |
| MOTA | 1549 | N | TYR A | 100 | | | 0.549 | 30.379 | 51.434 | 1.00 | 35.50 | 6 |
| ATOM | 1550 | CA | TYR A | 196 | | | 602 | 31.274 | 52.245 | 1.00 | 36.36 | 6 |
| ATOM | 1551 | CB | TYR A | 196 | | | | 31.816 | 53.538 | 1.00 | 37.28 | 6 |
| ATOM | 1552 | CG | TYR A | 196 | | | 175 | 32.848 | 53.527 | | 35.42 | 6 |
| ATOM | 1553 | CD1 | | | | | 1.120 | | 54.706 | | 33.10 | 6 |
| MOTA | 1554 | CEl | TYR A | 196 | | | 1.637 | 33.366 | 54.776 | | 36.75 | 6 |
| ATOM | 1555 | CD2 | TYR A | 196 | | | 9.764 | 31.311 | 55.968 | 1.00 | 35.26 | 6 |
| ATOM | 1556 | CE2 | TYR A | 196 | | | 0.279 | 31.825 | | | 35.84 | 6 |
| MOTA | 1557 | CZ | TYR A | 196 | | | 1.213 | 32.856 | 55.922 | 1.00 | 37.09 | 8 |
| ATOM | 1558 | ОН | TYR A | 196 | | 1: | 1.704 | 33.401 | 57.087 | 1.00 | 34.89 | 6 |
| MOTA | 1559 | C | TYR A | 196 | | | 1.878 | 31.097 | 51.188 | | | 8 |
| | 1560 | ō | TYR A | 196 | | 10 | 1.896 | 32.256 | 50.764 | 1.00 | 31.61 | 7 |
| ATOM | 1561 | N | ALA A | 197 | | | 2.991 | 30.416 | 51.437 | 1.00 | 34.39 | |
| MOTA | | CA | ALA A | 197 | | 14 | 4.297 | 31.041 | 51.242 | | 34.82 | 6 |
| MOTA | 1562 | | אבא ז | 197 | | | 4.684 | 31.826 | 52.489 | 1.00 | 32.48 | 6 |
| ATOM | 1563 | CB | ALA A | 107 | | | 5.418 | 30.075 | 50.887 | 1.00 | 36.59 | 6 |
| ATOM | 1564 | C | ALA A | 1 137 | | | 5.407 | 28.903 | 51.291 | | 37.46 | 8 |
| MOTA | 1565 | 0 | ALA | 197 | | | 6.388 | 30.584 | | 1.00 | 36.22 | 7 |
| MOTA | .1566 | N | PHE | A 198 | | | 7.548 | 29.802 | | 1.00 | 37.68 | 6 |
| ATOM | 1567 | ÇA | | A 198 | | | | 30.729 | | | 40.89 | 6 |
| ATOM | 1568 | CB | PHE A | A 198 | | | 8.597 | 30.723 | | | 43.59 | 6 |
| MOTA | 1569 | CG | PHE A | A 198 | | | 9.810 | 30.013 | | | 44.74 | 6 |
| ATOM | 1570 | CD1 | PHE A | A 198 | | | 9.783 | 29.404 | | | 41.86 | 6 |
| MOTA | 1571 | CD2 | PHE | A 198 | | | 0.970 | 29.929 | | | 41.42 | 6 |
| | 1572 | CE1 | PHE | A 198 | | | 0.894 | 28.729 | | | 43.30 | 6 |
| ATOM | 1573 | CEZ | PHE | A 198 | | 2 | 2.079 | 29.251 | | | 43.30 | 6 |
| ATOM | 1574 | CZ | PHE | A 198 | | | 2.040 | 28.652 | | | 41.86 | |
| MOTA | | c | DUE | A 198 | | 1 | 8.139 | 29.140 | | | 37.00 | 6 |
| MOTA | 1575 | | DUE. | A 198 | | | 8,166 | | 52.036 | | 36.43 | 8 |
| ATOM | 1576 | 0 | PRO | 3 100 | | | 8.641 | | 50.848 | | 37.63 | 7 |
| MOTA | 1577 | N | PRO | A 199 | | | 9.298 | | | 7 1.00 | 35.29 | 6 |
| MOTA | 1578 | CD | PRO | A 199 | | | 8.727 | | | 1.00 | 36.52 | 6 |
| ATOM | 1579 | | PRO | A 199 | | | | | | | 34.96 | 6 |
| ATOM | 1580 | | PRO | A 199 | | | 9.702 | | | | 34.57 | 6 |
| ATOM | 1581 | | PRO | A 199 | | | 9.281 | | | | 35.72 | |
| ATOM | 1582 | | PRO | A 199 | | | 17.409 | | | | 37.36 | |
| ATOM | 1583 | | PRO | A 199 | | | L7.386 | | · . | | 33.78 | |
| | | | PHE | A 200 | | 1 | 16.331 | 26.63 | 49.96 | 2 1.00 | | |
| ATOM | | - | | ٠. | | | | | | | | |

| ATOM | 1585 | CA PHE A 200 | | 15.004 | | 49.662 | 1.00 32.15 | 6 |
|--------------|--------------|-------------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 1586 | CB PHE A 200 | | 14.562 | 26.381 | 48.222 | 1.00 28.39 | 6 6 |
| ATOM | 1587 | CG PHE A 200 | | 14.600 | 27.827 | 47.835 | 1.00 26.29 1.00 24.82 | 6 |
| ATOM | 1588 | CD1 PHE A 200 | | 15.749 | 28.385 | 47.296 | 1.00 24.82 | 6 |
| ATOM | 1589 | CD2 PHE A 200 | | 13.466 | 28.623 | 47.966 | 1.00 25.68 | 6 |
| ATOM | 1590 | CE1 PHE A 200 | | 15.767 | 29.712 | 46.882 47.557 | 1.00 27.03 | 6 |
| ATOM | 1591 | CE2 PHE A 200 | | 13.475 | 29.955 | 47.013 | 1.00 24.90 | 6 . |
| ATOM | 1592 | CZ PHE A 200 | | 14.626 | 30.498 | 49.842 | 1.00 32.66 | 6 |
| MOTA | 1593 | C PHE A 200 | | 14.947 | 24.574 24.033 | 50.264 | 1.00 31.22 | 8 |
| ATOM | 1594 | O PHE A 200 | | 13.925 | 23.896 | 49.499 | 1.00 33.60 | 7 |
| MOTA | 1595 | N GLU A 201 | | 16.043 16.128 | 22.438 | 49.585 | 1.00 30.86 | 6 |
| ATOM | 1596 | CA GLU A 201 CB GLU A 201 | | 17.213 | 21.931 | 48.637- | 1.00 32.98 | 6 |
| MOTA | 1597 | | | 16.879 | 22.182 | 47.175 | 1.00 33.52 | 6 |
| MOTA | 1598 | CG GLU A 201 CD GLU A 201 | | 18.012 | 21.864 | 46.232 | 1.00 34.56 | 6 |
| MOTA | 1599 1600 | OE1 GLU A 201 | | 18.396 | 20.678 | 46.117 | 1.00 36.35 | 8 - |
| MOTA | 1601 | OE2 GLU A 201 | | 18.523 | 22.814 | 45.605 | 1.00 36.52 | 8 |
| MOTA MOTA | 1602 | C GLU A 201 | | 16.369 | 21.911 | 50.981 | 1.00 28.52 | 6 |
| MOTA | 1603 | O GLU A 201 | | 15.537 | 21.199 | 51.520 | 1.00 28.91 | 8 7 |
| ATOM | 1604 | N LYS A 202 | | 17.511 | 22.239 | 51.566 | 1.00 31.64 1.00 32.34 | 6 |
| ATOM | 1605 | CA LYS A 202 | | 17.795 | 21.780 | 52.917 | 1.00 32.34 | 6 |
| MOTA | 1606 | CB LYS A 202 | | 19.276 | 21.432 | 53.092 52.307 | 1.00 43.74 | 6 |
| ATOM | 1607 | CG LYS A 202 | | 19.789 | 20.226 | 50.891 | 1.00 49.31 | 6 |
| ATOM | 1608 | CD LYS A 202 | | 20.212 | 20.590 19.428 | 50.831 | 1.00 49.34 | 6 |
| MOTA | 1609 | CE LYS A 202 | | 20.952 21.504 | 19.428 | 48.895 | 1.00 49.89 | 7 |
| MOTA | 1610 | NZ LYS A 202 | | 17.421 | 22.849 | 53.937 | 1.00 30.55 | 6 |
| MOTA | 1611 | C LYS A 202 O LYS A 202 | | 16.877 | 23.890 | 53.586 | 1.00 26.55 | 8 |
| MOTA | 1612 | | • | 17.710 | 22.571 | 55.203 | 1.00 30.59 | 7 |
| MOTA | 1613 1614 | N GLY A 203 CA GLY A 203 | | 17.422 | 23.519 | 56.259 | 1.00 30.24 | 6 |
| ATOM | 1615 | C GLY A 203 | | 16.216 | 23.210 | 57.125 | 1.00 29.23 | 6 |
| ATOM ATOM | 1616 | O GLY A 203 | | 15.915 | 23.975 | 58.041 | 1.00 32.90 | 8 |
| ATOM | 1617 | N PHE A 204 | | 15.526 | 22.104 | 56.866 | 1.00 26.32 | 7 6 |
| MOTA | 1618 | CA PHE A 204 | | 14.344 | 21.779 | 57.657 | 1.00 23.25 1.00 21.25 | 6 |
| ATOM | 1619 | CB PHE A 204 | | 13.366 | 20.917 | 56.863 | 1.00 18.60 | 6 |
| ATOM | 1620 | CG PHE A 204 | | 12.855 | 21.573 | 55.635 54.461 | 1.00 16.43 | 6 |
| ATOM | 1621 | CD1 PHE A 204 | | 13.605 | 21.560 22.273 | 55.664 | 1.00 14.82 | 6 |
| ATOM | 1622 | CD2 PHE A 204 | | 11.654 13.168 | 22.245 | 53.333 | 1.00 16.91 | 6 |
| ATOM | 1623 | CE1 PHE A 204 | | 11.206 | 22.962 | 54.544 | 1.00 15.28 | 6 |
| ATOM | 1624 | CE2 PHE A 204 CZ PHE A 204 | | 11.965 | 22.952 | 53.375 | 1.00 18.34 | 6 |
| MOTA | 1625 | CZ PHE A 204 | | 14.626 | 21.094 | 58.979 | 1.00 23.72 | 6 |
| ATOM | 1626 1627 | O PHE A 204 | | 15.578 | 20.318 | 59.118 | 1.00 22.68 | 8 |
| ATOM | 1628 | N LEU A 205 | | 13.760 | 21.376 | 59.942 | 1.00 20.94 | 7 |
| MOTA MOTA | 1629 | CA LEU A 205 | | 13.877 | 20.818 | 61.272 | 1.00 24.83 | 6 6 |
| MOTA | 1630 | CB LEU A 205 | | 12.678 | 21.259 | 52.110 | 1.00 21.29 1.00 22.67 | 6 |
| ATOM | 1631 | CG LEU A 205 | | 12.672 | 20.811 | 33.568 | 1.00 22.07 | 6 |
| MOTA | 1632 | CD1 LEU A 205 | | 14.011 | 21.182 | 14.245 64.275 | 1.00 20.62 | 6 |
| ATOM | 1633 | CD2 LEU A 205 | | 11.478 | 21.456 19.293 | 61.303 | 1.00 28.79 | |
| MOTA | 1634 | C LEU A 205 | | 14.002 | 18.730 | 62.310 | 1.00 28.59 | 8 |
| MOTA | 1635 | 0 LEU A 205 | | 14.443 13.625 | 18.628 | 60.211 | 1.00 33.52 | 7 |
| ATOM | 1636 | N GLU A 200 | | 13.693 | 17.166 | 60.142 | 1.00 39.79 | 6 |
| MOTA | 1637 | CA GLU A 200 CB GLU A 200 | | 12.736 | 16.616 | 59.070 | 1.00 44.37 | 6 |
| MOTA | 1638 | CB GLU A 200 | | 11.284 | 17.060 | 59.204 | 1.00 50.75 | 6 |
| ATOM | 1639 1640 | CD GLU A 20 | | 11.014 | 18.390 | 58.512 | 1.00 55.31 | 6 |
| ATOM | 1641 | OE1 GLU A 20 | | 9.972 | 19.027 | 58.797 | 1.00 55.36 | 8 |
| MOTA | 1642 | OE2 GLU A 20 | | 11.839 | 18.786 | 57.661 | 1.00 56.48 | 8 |
| MOTA MOTA | 1643 | C GLU A 20 | 5 | 15.114 | 16.674 | 59.847 | | 6 8 |
| ATOM | 1644 | 0 GLU A 20 | | 15.483 | 15.541 | 60.180 | | 7 |
| ATOM | 1645 | N GLU A 20 | 7 | 15.903 | | 59.217 | | 6 |
| MOTA | 1646 | CA GLU A 20 | 7 | 17.286 | | 58.873 | | 6 |
| MOTA | 1647 | CB GLU A 20 | 7 | 17.776 | | 57.854 56.556 | | 6 |
| ATOM | 1648 | CG GLU A 20 | 7 | 16.983 | | | | 6 |
| ATOM | 1649 | CD GLU A 20 | 7 | 16.978 | 19.452 | | | 8 |
| MOTA | 1650 | OE1 GLU A 20 | ′ | 18.071 | 20.016 | - | | |
| | | | • | | | | | |

| | | | | | | | | 8 |
|------|---------|-----|-------------|--------|----------|--------|------------|-----|
| | 1 (5) | 023 | GLU A 207 | 15.870 | 19.891 | 55.389 | 1.00 34.62 | |
| ATOM | 1651 | | | 18.139 | 17.239 | 60.134 | 1.00 36.18 | 6 |
| MOTA | 1652 | | GLU A 207 | | | 60.590 | 1.00 34.81 | 8 |
| ATOM | 1653 | 0 | GLU A 207 | 18.560 | 18.303 | | | 7 |
| | | | ILE A 208 | 18.381 | 16.059 | 60.701 | 1.00 34.45 | |
| ATOM | 1654 | N | 1LE A 200 | 19.164 | 15.965 | 61.932 | 1.00 38.53 | 6 |
| ATOM | 1655 | CA | ILE A 208 | | | | 1.00 41.12 | 6 |
| | 1656 | CB | ILE A 208 | 18.260 | 15.511 | 63.117 | | |
| ATOM | | | ILE A 208 | 19.097 | 15.273 | 64.375 | 1.00 41.36 | 6 |
| ATOM | 1657 | CG2 | 1LE A 200 | | 16.581 | 63.383 | 1.00 42.21 | 6 |
| MOTA | 1658 | CG1 | ILE A 208 | 17.193 | | | 1.00 44.81 | 6 |
| | 1659 | CD1 | ILE A .208 | 16.291 | 16.286 | 64.560 | | |
| ATOM | | | | 20.407 | 15.074 | 61.876 | 1.00 36.66 | 6 |
| MOTA | 1660 | Ç | ILE A 208 | | | 62.775 | 1.00 34.03 | 8 |
| MOTA | 1661 | 0 | ILE A 208 | 21.243 | 15.110 | | 1.00 36.80 | 7 |
| | | N | GLY A 209 | 20.540 | 14.284 | 60.822 | | |
| ATOM | 1662 | | GE1 1. 200 | 21.703 | 13.428 | 60.728 | 1.00 38.99 | 6 |
| ATOM | 1663 | CA | GLY A 209 | | | 59.805 | 1.00 40.93 | 6 |
| MOTA | 1664 | C | GLY A 209 | 21.509 | 12.246 | | 1.00 40.26 | 8 |
| | 1665 | ō | GLY A 209 | 20.477 | 12.124 | 59.145 | | |
| MOTA | | | | 22.508 | 11.370 | 59.775 | 1.00 42.16 | 7 |
| ATOM | 1666 | N | GLU A 210 | | | 58.930 | 1.00 43.30 | 6 |
| MOTA | 1667 | CA | GLU A 210 | 22.492 | 10.185 | 50.350 | 1.00 47.08 | 6 |
| | 1668 | CB | GLU A 210 | 22.810 | 10.586 | 57.488 | 1.00 47.08 | |
| MOTA | | | GLU A 210 | 22.826 | 9.453 | 56.478 | 1.00 53.90 | 6 |
| MOTA | 1669 | CG | GLU A 210 | | 9.915 | 55.089 | 1.00 56.27 | 6 |
| ATOM | 1670 | CD | GLU A 210 | 23.256 | | | 1.00 56.19 | 8 |
| | 1671 | OE1 | | 24.412 | 10.371 | 54.941 | | |
| MOTA | _ | | | 22.437 | 9.826 | 54.145 | 1.00 60.28 | 8 |
| ATOM | 1672 | OE2 | | | 9.276 | 59.473 | 1.00 41.47 | 6 |
| MOTA | 1673 | С | GLU A 210 | 23.583 | | | 1.00 43.97 | 8 |
| | 1674 | Ō | GLU A 210 | 24.750 | 9.457 | 59.152 | | |
| MOTA | | | GLY A 211 | 23.203 | 8.307 | 60.299 | 1.00 39.97 | 7 |
| ATOM | 1675 | N | | | 7.405 | 60.885 | 1.00 37.34 | 6 |
| MOTA | 1676 | CA | GLY A 211 | 24.181 | | | 1.00 37.84 | 6 |
| | 1677 | Ċ | GLY A 211 | 24.642 | 7.952 | 62.224 | 1.00 37.04 | |
| MOTA | | | GLY A 211 | 23.820 | 8.408 | 63.019 | 1.00 37.30 | 8 |
| MOTA | 1678 | 0 | | 25.948 | | 62.485 | 1.00 38.52 | 7 |
| ATOM | 1679 | N | LYS A 212 | | | | 1.00 38.29 | 6 |
| | 1680 | CA | LYS A 212 | 26.490 | 8.440 | 63.733 | | |
| MOTA | - | | LYS A 212 | 28.020 | 8.359 | 63.731 | 1.00 40.54 | 6 |
| MOTA | 1681 | CB | LIS A 212 | 28.570 | | 63:675 | 1.00 46.39 | 6 |
| MOTA | 1682 | CG | LYS A 212 | | | | 1.00 51.59 | 6 |
| | 1683 | CD | LYS A 212 | 28.149 | 6.147 | 64.910 | 1.00 51.33 | |
| MOTA | | | LYS A 212 | 28.556 | 4.676 | 64.809 | 1.00 52.77 | 6 |
| ATOM | 1684 | CE | DIS A 212 | 30.030 | 4.478 | 64.662 | 1.00 55.48 | 7 |
| ATOM | 1685 | ΝZ | LYS A 212 | | | 63.866 | 1.00 37.68 | 6 |
| ATOM | 1686 | С | LYS A 212 | 26.061 | | | 1.00 37.00 | |
| | | ō | LYS A 212 | 25.814 | 10.389 | 64.962 | 1.00 34.75 | |
| MOTA | 1687 | | | 25.956 | | 62.728 | 1.00 38.89 | 7 |
| ATOM | 1688 | N | GLY A 213 | | | 62.724 | 1.00 43.58 | 6 |
| MOTA | 1689 | CA | GLY A 213 | 25.577 | | | 1.00 43.99 | 6 |
| _ | 1690 | С | GLY A 213 | 24.126 | 12.295 | 63.020 | | |
| MOTA | | | GLY A 213 | 23.737 | | 63.024 | 1.00 44.67 | 8 |
| ATOM | 1691 | С | GLY M 213 | 22.727 | | 63.265 | 1.00 46.02 | 7 |
| ATOM | 1692 | N | LYS A 214 | 23.321 | | | 1.00 45.61 | 6 |
| | 1693 | CA | LYS A 214 | 21.907 | 11.467 | 63.562 | | 6 |
| ATOM | | | LYS A 214 | 21.168 | 10.130 | 63.469 | 1.00 47.77 | |
| ATOM | 1694 | CB | LIS A 214 | 19.675 | | | 1.00 49.25 | 6 |
| MOTA | 1695 | CG | LYS A 214 | | | | 1.00 51.64 | 6 |
| | 1696 | CD | LYS A 214 | 19.078 | | | 1.00 52.00 | 6 |
| MOTA | 1607 | CE | LYS A 214 | 17.637 | 9.038 | 62.440 | 1.00 54.30 | |
| MOTA | 1697 | | 110 h 214 | 17.030 | | | 1.00 56.09 | 7 |
| MOTA | 1698 | NZ | LYS A 214 | | | | 1.00 44.22 | 6 |
| ATOM | 1699 | С | LYS A 214 | 21.809 | | | 1.00 45.04 | 8 |
| | | | LYS A 214 | 22.210 |) 11.410 | 65.942 | | |
| MOTA | 1700 | | 010 11 21 5 | 21.292 | | 65.074 | 1.00 42.89 | 7 |
| MOTA | 1701 | N | GLY A 215 | | | | 1.00 40.20 | 6 |
| MOTA | 1702 | CA | GLY A 215 | 21.193 | | | | 6 |
| | | C | GLY A 215 | 22.295 | 14.931 | 66.600 | | |
| MOTA | 1703 | | ON A 015 | 22.356 | | | 1.00 40.12 | 8 |
| ATOM | 1704 | 0 | GLY A 215 | | | | 10 | 7 |
| ATOM | 1705 | N | TYR A 216 | 23.175 | | | | 6 |
| | 1706 | | | 24.263 | 16.086 | 65.726 | | |
| ATOM | - | | | 25.632 | | | 1.00 36.47 | 6 |
| ATOM | 1707 | CB | | | | | | 6 |
| ATOM | 1708 | CG | TYR A 216 | 25.93 | | | | 6 |
| | | | 1 TYR A 216 | 25.29 | 5 13.220 | 66.810 | | |
| MOTA | 1709 | | | 25.56 | | | 1.00 41.58 | 6 |
| ATOM | 1710 | | | | | | | 6 |
| ATOM | 1711 | CD | 2 TYR A 216 | 26.85 | | | | 6 |
| | | | | 27.12 | 4 13.919 | 68.786 | | |
| ATOM | 1712 | | | 26.47 | | | 1.00 41.86 | 6 |
| ATOM | 1713 | | | | | | 1.00 43.04 | 8 |
| ATOM | 1714 | OH | TYR A 216 | 26.74 | | | | · 6 |
| | | | TYR A 216 | 24.18 | 2 17.21 | | | 8 |
| atom | 1715 | | | 25.19 | | | 1.00 33.37 | 0 |
| ATOM | 1716 | , 0 | TYR A 216 | 23.23 | | • | | |

| | | | 2 217 | | 22 | 976 | 17.471 | 64.212 | 1.00 33.83 | 7 |
|--------------|--------------|----------|------------------------|---|-----|-------|--------|----------------------|--------------|--------|
| MOTA | | N | ASN A 217 | | 22. | 726 | 18.558 | 63.267 | 1.00 30.20 | 6 |
| MOTA | | CA | ASN A 217 | | | . 699 | 18.057 | 61.823 | 1.00 27.74 | 6 |
| ATOM | | | ASN A 217 | | | 457 | 19.177 | 60.826 | 1.00 25.61 | 6 |
| MOTA | | CG | ASN A 217 | | | . 354 | 19.705 | 60.719 | 1.00 25.00 | 8 |
| MOTA | | OD1 | ASN A 217 | | | | 19.558 | 60.103 | 1.00 30.43 | 7 |
| MOTA | 1722 | ND2 | ASN A 217 | | | . 501 | 19.116 | 63.645 | 1.00 29.09 | 6 |
| ATOM | 1723 | С | ASN A 217 | | | . 369 | 18.351 | 63.885 | 1.00 26.93 | 8 |
| ATOM | 1724 | | ASN A 217 | | | . 433 | 20.440 | 63.710 | 1.00 27.19 | 7 |
| ATOM | 1725 | | LEU A 218 | | | . 263 | 21.071 | 64.089 | 1.00 25.33 | 6 |
| ATOM | 1726 | CA | LEU A 218 | | | .010 | 21.071 | 65.590 | 1.00 23.23 | 6 |
| ATOM | 1727 | CB | LEU A 218 | | | .026 | 21.704 | 66.346 | 1.00 21.00 | 6 |
| MOTA | 1728 | CG | LEU A 218 | | | .729 | 22.313 | 67.695 | 1.00 18.62 | 6 |
| MOTA | 1729 | CD1 | LEU A 218 | • | | .100 | 22.313 | 65.583 | 1.00 18.48 | 6 |
| ATOM | 1730 | CD2 | LEU A 218 | | | .872 | 22.368 | 63.325 | 1.00 25.04 | 6 |
| MOTA | 1731 | С | LEU A 218 | | | .785 | 23.287 | 63.415 | 1.00 25.23 | 8 |
| ATOM | 1732 | 0 | LEU A 218 | | | .596 | 22.436 | 62.584 | 1.00 28.44 | 7 |
| ATOM | 1733 | N | ASN A 219 | | 18 | .681 | 23.636 | 61.829 | 1.00 28.76 | 6 |
| ATOM | 1734 | CA | ASN A 219 | | | .310 | 23.298 | 60.417 | 1.00 25.69 | 6 |
| ATOM | 1735 | CB | ASN A 219 | | _ | .809 | 22.408 | 59.646 | 1.00 26.10 | 6 |
| ATOM | 1736 | CG | ASN A 219 | | | .748 | 22.708 | 59.505 | 1.00 28.53 | 8 |
| MOTA | 1737 | OD1 | ASN A 219 | | | .927 | 21.311 | 59.114 | 1.00 26.97 | 7 |
| MOTA | 1738 | | ASN A 219 | | | .220 | 24.248 | 62.582 | 1.00 31.96 | 6 |
| MOTA | 1739 | С | ASN A 219 | | | .129 | 23.539 | 63.246 | 1.00 34.84 | 8 |
| ATOM | 1740 | Ο. | ASN A 219 | | | .952 | 25.556 | 62.472 | 1.00 32.96 | 7 |
| MOTA | 1741 | N | ILE A 220 | | | .826 | 26.196 | 63.129 | 1.00 32.50 | 6 |
| ATOM | 1742 | CA | ILE A 220 | | | .259 | 27.037 | 64.350 | 1.00 32.32 | 6 |
| MOTA | 1743 | CB | ILE A 220 | | | .029 | 27.644 | 65.014 | 1.00 29.46 | 6. |
| MOTA | 1744 | CG2 | ILE A 220 | | | .978 | 26.160 | 65.374 | 1.00 29.65 | 6 |
| MOTA | 1745 | CG1 | ILE A 220 | | | .080 | 25.138 | 66.027 | 1.00 28.65 | 6 |
| MOTA | 1746 | CD1 | ILE A 220 ILE A 220 | | | .140 | 27.106 | 62.123 | 1.00 35.36 | 6 |
| MOTA | 1747 | C | ILE A 220 | | | .469 | 28.290 | 62.009 | 1.00 35.52 | 8 |
| MOTA | 1748 | 0 | PRO A 221 | | | 1.185 | 26.553 | 61.359 | 1.00 36.87 | 7 |
| MOTA | 1749 | N | PRO A 221 | | | 3.718 | 25.158 | 61.359 | 1.00 35.12 | 6 |
| ATOM | 1750 | CD | PRO A 221 | | | 3.445 | 27.318 | 60.356 | 1.00 35.41 | 6 |
| MOTA | 1751 | CA | PRO A 221 | | | 2.509 | 26.262 | 59.767 | 1.00 35.68 | 6 |
| ATOM | 1752 | CB CG | PRO A 221 | | | 3.319 | 24.992 | 59.911 | 1.00 33.86 | 6 |
| MOTA | 1753 | C | PRO A 221 | | | 2.696 | 28.437 | 61.053 | 1.00 34.37 | 6 |
| MOTA | 1754 1755 | o | PRO A 221 | | | 2.014 | 28.199 | 62.043 | 1.00 38.79 | 8 7 |
| ATOM | 1756 | N | LEU A 222 | | 13 | 2.815 | 29.655 | 60.547 | 1.00 34.76 | 6 |
| ATOM | 1757 | CA | LEU A 222 | | 13 | 2.138 | 30.796 | 61.166 | 1.00 33.87 | 6 |
| ATOM | 1758 | CB | LEU A 222 | | 1 | 3.173 | 31.735 | 61.798 | 1.00 35.13 | 6 |
| MOTA | 1759 | CG | LEU A 222 | | 1 | 4.104 | 31.163 | | 1.00 33.07 | 6 |
| ATOM ATOM | 1760 | CD1 | LEU A 222 | | 1 | 5.234 | 32.150 | | 1.00 34.04 | 6 |
| ATOM | .1761 | CD2 | LEU A 222 | | 1 | 3.312 | 30.856 | | | 6 |
| ATOM | 1762 | С | LEU A 222 | | | 1.287 | 31.567 | | | 8 |
| ATOM | 1763 | 0 | LEU A 222 | | | 1.669 | 31.740 | | | 7 |
| ATOM | 1764 | N | PRO A 223 | | | 0.127 | 32.060 | | | 6 |
| MOTA | 1765 | CD | PRO A 223 | | | 9.606 | 31.913 | | | 6 |
| ATOM | 1766 | CA | PRO A 223 | | | 9.173 | 32.818 | | | 6 |
| MOTA | 1767 | CB | PRO A 223 | | | 7.957 | | | | 6 |
| ATOM | 1768 | ÇG | PRO A 223 | | | 8.626 | | | | 6 |
| ATOM | 1769 | С | PRO A 223 | | | 9.645 | | | | 8 |
| MOTA | 1770 | 0 | PRO A 223 | | 1 | 0.694 | | | | 7 |
| ATOM | 1771 | N | LYS A 224 | | | 8.841 | | | | |
| ATOM | 1772 | CA | LYS A 224 | | | 9.115 | 36.172 | 2 58.026 3 56.766 | | 6 |
| ATOM | 1773 | CB | LYS A 224 | | | 8.285 | | | | 6 |
| ATOM | 1774 | CG | LYS A 224 | | | 8.563 | | | | |
| MOTA | 1775 | CD | LYS A 224 | | | 7.737 | | | | |
| ATOM | 1776 | CE | LYS A 224 | | | 8.065 | 34.769 | | | |
| ATOM | 1777 | NZ | LYS A 224 | | | 7.198 | | | | |
| ATOM | 1778 | C | LYS A 224 | | | 8.702 | | 59.113 | | |
| ATOM | 1779 | | LYS A 224 | | | 7.999 | | | | |
| ATOM | 1780 | | GLY A 225 | | | 9.124 | | | | |
| ATOM | 4-04 | | | | | 8.777 | | | | |
| AIOM | 1782 | | GLY A 225 | | | 9.396 | 39.18 | 8 61.28 | 0 1.00 32,30 | |

| | | O GLY A 225 | | 9.068 | 39.861 | 62.271 | 1.00 31.20 | 8 |
|--------------|--------------|-------------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| MOTA | | | | 10.299 | 38.216 | 61.338 | 1.00 32.86 | 7 |
| MOTA | | 226 | | 10.975 | 37.877 | 62.575 | 1.00 34.55 | 6 |
| MOTA | | | | 12.149 | 36.958 | 62.255 | 1.00 34.46 | 6 |
| ATOM | | | | 12.982 | 36.413 | 63.407 | 1.00 34.48 | 6 |
| ATOM | | CG LEU A 226 CD1 LEU A 226 | | 12.146 | 35.425 | 64.212 | 1.00 33.18 | 6 |
| ATOM | 1788 | CDI LEU A 220 | | 14.207 | 35.724 | 62.847 | 1.00 31.39 | 6 |
| MOTA | _ | CD2 LEU A 226 C LEU A 226 | | 11.481 | 39.160 | 63.255 | 1.00 36.29 | 6 |
| MOTA | | | | 12.156 | 39.970 | 62.613 | 1.00 33.87 | 8 |
| MOTA | 1791 | O LEU A 226 | | 11.131 | 39.358 | 64.531 | 1.00 37.31 | 7 |
| MOTA | 1792 | N ASN A 227 | | 11.592 | 40.536 | 65.279 | 1.00 37.26 | 6 |
| ATOM | 1793 | CA ASN A 227 CB ASN A 227 | | 10.444 | 41.212 | 66.053 | 1.00 35.57 | 6 |
| MOTA | 1794 | | | 9.920 | 40.368 | 67.208 | 1.00 36.07 | 6 |
| MOTA | 1795 | OD1 ASN A 227 | | 10.678 | 39.940 | 68.089 | 1.00 35.08 | 8 |
| MOTA | 1796 | ND2 ASN A 227 | | 8.611 | 40.143 | 67.218 | 1.00 32.33 | 7 |
| MOTA | 1797 | | | 12.688 | 40.096 | 66.259 | 1.00 37.95 | 6 |
| ATOM | 1798 | | • | 12.869 | 38.890 | 66.473 | 1.00 37.08 | 8 |
| MOTA | 1799 | | | 13.403 | 41.063 | 66.832 | 1.00 36.07 | 7 |
| MOTA | 1800 | N ASP A 228 CA ASP A 228 | | 14.505 | 40.754 | 67.751 | 1.00 37.63 | 6 |
| ATOM | 1801 | 000 | | 14.996 | 42.007 | 68.486 | 1.00 36.48 | 6 |
| MOTA | 1802 | CB ASP A 228 | | 15.480 | 43.088 | 67.545 | 1.00 37.52 | 6 |
| ATOM | 1803 1804 | OD1 ASP A 228 | | 15.936 | 42.752 | 66.427 | 1.00 35.28 | 8 |
| MOTA | | OD2 ASP A 228 | | 15.426 | 44.274 | 67.937 | 1.00 39.01 | 8 |
| MOTA | 1805 | C ASP A 228 | | 14.204 | 39.678 | 68.783 | 1.00 37.56 | 6 |
| MOTA | 1806 1807 | O ASP A 228 | | 14.921 | 38.678 | 68.869 | 1.00 39.53 | 8 |
| MOTA | 1808 | N ASN A 229 | | 13.155 | 39.889 | 69.572 | 1.00 38.37 | 7 |
| MOTA | 1809 | CA ASN A 229 | | 12.766 | 38.935 | 70.605 | 1.00 37.49 | 6 |
| MOTA | 1810 | CB ASN A 229 | | 11.422 | 39.352 | 71.200 | 1.00 37.38 | 6 |
| ATOM | 1811 | CG ASN A 229 | | 11.490 | 40.709 | 71.877 | 1.00 40.47 | 6 |
| ATOM ATOM | 1812 | OD1 ASN A 229 | | 12.041 | 40.840 | 72.973 | 1.00 41.76 | 8 |
| MOTA | 1813 | ND2 ASN A 229 | | 10.960 | 41.735 | 71.212 | 1.00 36.50 | 7 6 |
| MOTA | 1814 | C ASN A 229 | | 12.680 | 37.530 | 70.017 | 1.00 37.64 1.00 35.76 | 8 |
| ATOM | 1815 | O ASN A 229 | | 13.446 | 36.634 | 70.395 | | 7 |
| ATOM | 1816 | N GLU A 230 | | 11.758 | 37.351 | 69.076 | 1.00 36.01 1.00 34.74 | 6 |
| MOTA | 1817 | CA GLU A 230 | | 11.574 | 36.062 | 68.425 | 1.00 34.74 | 6 |
| ATOM | 1818 | CB GLU A 230 | | 10.753 | 36.242 | 67.153 | 1.00 36.95 | 6 |
| ATOM | 1819 | CG GLU A 230 | | 9.382 | 36.820 | 67.407 66.144 | 1.00 35.30 | 6 |
| ATOM | 1820 | CD GLU A 230 | | 8.580 | 36.960 | 65.229 | 1.00 36.98 | 8 |
| ATOM | 1821 | OE1 GLU A 230 | | 9.042 | 37.670 | 66.065 | 1.00 36.71 | 8 |
| MOTA | 1822 | OE2 GLU A 230 | | 7.490 | 36.361 | 68.082 | 1.00 33.92 | 6 |
| ATOM | 1823 | C GLU A 230 | | 12.916 | 35.421 34.238 | 68.346 | 1.00 32.74 | 8 |
| ATOM | 1824 | O GLU A 230 | | 13.143 | 36.207 | 67.487 | 1.00 32.03 | 7 |
| ATOM | 1825 | N PHE A 231 | | 13.804 | 35.712 | 67.123 | 1.00 30.55 | 6 |
| ATOM | 1826 | CA PHE A 231 | | 15.116 | 36.821 | 66.460 | 1.00 33.86 | 6 |
| MOTA | 1827 | СВ РНЕ А 231 | | 15.932 | | 66.012 | 1.00 36.97 | 6 |
| MOTA | 1828 | CG 'HE A 231 | | 17.295 17.438 | | 65.102 | | 6 |
| MOTA | 1829 | CD1 HE A 231 | | 18.436 | 37.021 | 66.480 | 1.00 36.58 | 6 |
| MOTA | 1830 | CD2 .HE A 231 | | 18.709 | 34.932 | 64.661 | 1.00 43.00 | 6 |
| MOTA | 1831 | CE1 PHE A 231 | | 19.711 | 36.632 | 66.049 | 1.00 39.07 | 6 |
| MOTA | 1832 | CE2 PHE A 231 | | 19.849 | 35.586 | 65.137 | 1.00 40.52 | 6 |
| MOTA | 1833 | CZ PHE A 231 | | 15.835 | | 68.376 | 1.00 30.63 | 6 |
| ATOM | 1834 | C PHE A 231 | | 16.177 | | 68.497 | 1.00 29.66 | 8 |
| MOTA | 1835 | O PHE A 231 | | 16.049 | | | 1.00 24.94 | 7 |
| MOTA | 1836 | N LEU A 232 | | 16.742 | | 70.556 | 1.00 22.82 | 6 |
| MOTA | 1837 | CA LEU A 232 | | 16.724 | | 71.468 | | 6 |
| MOTA | 1838 | CB LEU A 232 | | 17.507 | _ | 70.890 | 1.00 29.34 | 6 |
| ATOM | 1839 | CG LEU A 232 | | 17.316 | | 71.746 | 1.00 24.38 | 6 |
| MOTA | 1840 | CD1 LEU A 232 | | 18.991 | | 70.787 | 1.00 27.39 | 6 |
| ATOM | 1841 | CD2 LEU A 232 | | 16.150 | | | 1.00 22.44 | 6 |
| ATOM | 1842 | C LEU A 232 | | 16.882 | | | | 8 |
| MOTA | 1843 | O LEU A 232 | | 14.825 | | | 1.00 24.81 | 7 |
| MOTA | 1844 | N PHE A 233 | | 14.131 | | | 1.00 25.81 | 6 |
| MOTA | 1845 | CA PHE A 233 | | 12.623 | _ | 71.641 | 1.00 24.37 | 6 |
| MOTA | 1846 | CB PHE A 233 | | 11.81 | | | 1.00 24.18 | 6 |
| MOTA | 1847 | CG PHE A 233 | | 11.491 | | | 1.00 25.59 | 6 |
| MOTA | 1848 | CD1 PHE A 233 | | 11.47 | | • | • | |

| | • | | _ | | | | | |
|---|--|--|---|---|--|--|--|---|
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 1850 1851 1852 1853 1854 1855 | CA GLU A 240 CB GLU A 240 CG GLU A 240 | | 11.339 10.698 10.548 10.548 14.661 15.094 14.624 15.080 14.797 16.563 18.789 19.548 21.039 21.625 21.803 18.974 19.648 18.347 17.843 16.610 15.686 16.988 17.363 18.767 18.3767 18.3767 16.138 18.7767 16.138 14.791 12.712 12.315 17.455 18.479 17.455 18.479 17.455 17.455 18.479 19.664 20.367 21.663 22.620 22.620 23.663 22.620 23.663 22.6293 22 | 27.914 29.087 30.189 28.681 25.666 24.764 25.835 24.965 25.369 | 73.974 71.747 73.093 71.747 73.093 71.275 71.971 69.209 67.720 69.438 69.769 69.703 69.316 69.703 69.317 71.312 72.192 73.561 74.452 74.635 74.843 75.184 75.183 76.083 77.085 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 77.099 | 1.00 24.31 1.00 24.63 1.00 23.11 1.00 31.99 1.00 32.57 1.00 33.86 1.00 38.61 1.00 43.21 1.00 53.52 | 666668766687666668766668868766666768766888766876666 |
| MOTA | 1897 | CD2 LEU A 239 | | 23.663 21.463 | 28.681 25.666 | 73.275 | 1.00 31.99 | 6 |
| MOTA | 1899 | O LEU A 239 | | 22.279 | 24.764 | | 1.00 33.86 | 7 |
| | 1900 | CA GLU A 240 | | 20.094 | 24.965 | 75.136 | | |
| ATOM | 1902 | | | | 24.468 | 77.045 | 1.00 53.52 | |
| atom atom | 1903 | CD GLU A 240 | | 19.677 | 24.383 | | | 8 |
| ATOM | 1905 | OE1 GLU A 240 | | 19.969 20.318 | 25.399 3 23.304 | | 1.00 55.12 | 8 |
| MOTA | 1906 | | | 20.033 | | 74.722 | 1.00 39.28 | 6 |
| MOTA | 1907 1908 | | | 20.532 | 2 22.63 | 75.437 | | 8 7 |
| ATOM ATOM | 1908 | N ILE A 241 | | 19.423 | 3 23.25 | | | 6 |
| ATOM | 1910 |) CA ILE A 241 | | 19.310 | | | 1.00 33.57 | 6 |
| ATOM | 1911 | CB ILE A 241 | | 18.465 18.53 | | | 6 1.00 31.39 | . 6 |
| ATCM | | | | 17.01 | 2 22.22 | 6 72.05 | 6 1.00 31.06 | · 6 |
| ATOM | | | | 16.14 | | 8 70.84 | 3 1.00 27.53 | 0 |
| MOTA | ニフエマ | | | | | - | | |

| | | | | • | | | | | | _ |
|------|------|------|------------|----------|------|-------|--------|----------|-------------|------|
| | 1015 | _ | ILE A 241 | 1 | 20.7 | 13 | 21.372 | 72.747 | 1.00 39.56 | 6 |
| atom | 1915 | C | TLE A 241 | <u>.</u> | 20.9 | | 20.189 | 72.936 | 1.00 40.82 | 8 |
| ATOM | 1916 | 0 | ILE A 241 | L | | | 22.254 | 72.299 | 1.00 41.93 | 7 |
| MOTA | 1917 | N | VAL A 242 | 2 | 21.6 | | | | 1.00 45.09 | 6 |
| | 1918 | CA | VAL A 242 | 2 | 22.9 | | 21.842 | 72.015 | | |
| ATOM | | | VAL A 242 | | 23.8 | 08 | 22.959 | 71.329 | 1.00 45.76 | 6 |
| MOTA | 1919 | CB | VAL A 244 | - | 25.2 | | 22.479 | 71.116 | 1.00 43.09 | 6 |
| ATOM | 1920 | CG1 | VAL A 242 | 2 | | | | 69.991 | 1.00 46.41 | 6 |
| ATOM | 1921 | CG2 | VAL A 242 | 2 | 23.1 | | 23.334 | | | 6 |
| | 1922 | С | VAL A 242 | 2 | 23.6 | 98 | 21.453 | 73.300 | 1.00 45.69 | |
| ATOM | | | VAL A 24 | 2 | 24.1 | 91 | 20.331 | 73.423 | 1.00 46.30 | 8 |
| ATOM | 1923 | 0 | VAD A 244 | 2 | 23.7 | | 22.373 | 74.259 | 1.00 44.60 | 7 |
| ATOM | 1924 | N | LYS A 24 | . | | | 22.088 | 75.513 | 1.00 46.96 | 6 |
| MOTA | 1925 | ÇA | LYS A 24 | 3 | 24.4 | | | | 1.00 49.49 | 6 |
| ATOM | 1926 | CB | LYS A 24 | 3 | 24.2 | 14 | 23.217 | 76.527 | | 6 |
| | 1927 | CG | LYS A 24 | 3 | 25.0 | 61 | 23.023 | 77.795 | 1.00 54.90 | |
| ATOM | | | LYS A 24 | - 3 | 24.6 | 52 | 23.934 | 78.939 | 1.00 58.95 | 6 |
| ATOM | 1928 | CD | DIS A 24 | - - | 24.7 | | 25.399 | 78.577 | 1.00 64.13 | 6 |
| MOTA | 1929 | CE | LYS A 24 | | | | 26.283 | 79.676 | 1.00 66.93 | 7 |
| ATOM | 1930 | NZ | LYS A 24 | 3 | 24.2 | | | | 1.00 47.06 | 6 |
| | 1931 | С | LYS A 24 | 3 | 23.9 | 65 | 20.767 | 76.135 | 1.00 47.00 | 8 |
| MOTA | 1932 | ō | LYS A 24 | 3 | 24.7 | 735 | 20.113 | 76.845 | 1.00 46.39 | |
| MOTA | | | GLU A 24 | <u> </u> | 22.7 | 716 | 20.380 | 75.878 | 1.00 47.51 | 7 |
| MOTA | 1933 | N | GLU A 24 | 7 | 22.1 | | 19.136 | 76.429 | 1.00 51.33 | 6 |
| MOTA | 1934 | CA | GLU A 24 | 4 | | | 19.061 | 76.259 | 1.00 54.49 | 6 |
| MOTA | 1935 | CB | GLU A 24 | | 20.6 | | | | 1.00 62.61 | 6 |
| ATOM | 1936 | CG | GLU A 24 | 4 | 19.8 | 343 | 20.199 | 76.842 | 1.00 02.01 | |
| | 1937 | CD | GLU A 24 | | 18.3 | 360 | 20.089 | 76.489 | 1.00 65.15 | 6 |
| ATOM | | | | | 17.5 | 572 | 20.980 | 76.888 | 1.00 66.49 | |
| MOTA | 1938 | OE1 | | | 17.9 | | 19.108 | 75.807 | 1.00 64.82 | 8 |
| ATOM | 1939 | OE2 | | | | | 17.936 | 75.698 | 1.00 50.17 | 6 |
| MOTA | 1940 | С | GLU A 24 | | 22. | | | | 1.00 51.54 | |
| ATOM | 1941 | 0 | GLU A 24 | 4 | 22.1 | 866 | 16.846 | 76.259 | | |
| | 1942 | N | VAL A 24 | | 23. | 104 | 18.148 | 74.441 | 1.00 47.70 | |
| MOTA | | | VAL A 24 | | 23. | 587 | 17.063 | 73.611 | 1.00 45.43 | |
| MOTA | 1943 | CA | | | 22. | | 16.980 | 72.336 | 1.00 48.47 | 6 |
| ATOM | 1944 | CB | VAL A 24 | | | | 15.765 | 71.499 | 1.00 51.87 | 6 |
| MOTA | 1945 | CG1 | VAL A 24 | | 23. | | | 72.731 | 1.00 45.65 | 6 |
| MOTA | 1946 | CG2 | VAL A 24 | 15 | 21. | 226 | 16.934 | | 1.00 43.01 | |
| | 1947 | С | VAL A 24 | 15 | 25. | 056 | 17.070 | 73.185 | | |
| MOTA | | | VAL A 24 | | 25. | 620 | 16.005 | 72.946 | 1.00 39.28 | 8 |
| ATOM | 1948 | 0 | AVD V 54 | 16 | 25. | | 18.245 | 73.109 | 1.00 40.53 | 7 |
| ATOM | 1949 | N | PHE A 24 | | | | 18.321 | 72.633 | 1.00 38.56 | 5 6 |
| ATOM | 1950 | CA | PHE A 24 | | 27. | | | 71.154 | 1.00 36.85 | 6 |
| ATOM | 1951 | CB | PHE A 24 | 16 | 27. | | 18.700 | | | _ |
| | 1952 | CG | PHE A 24 | 16 | 28. | | 18.487 | 70.415 | | |
| ATOM | | CD1 | PHE A 24 | | 28. | 749 | 17.201 | 70.098 | 1.00 32.95 | _ |
| MOTA | 1953 | | | 16 | | 064 | 19.582 | 69.967 | 1.00 35.53 | 6 |
| ATOM | 1954 | CD2 | | | | 903 | 17.004 | 69.337 | 1.00 33.80 |) 6 |
| ATOM | 1955 | CE: | | | | | 19.397 | 69.206 | 1.00 34.46 | 66 |
| MOTA | 1956 | CE | 2 PHE A 24 | 46 | | 222 | | | 1.00 35.5 | |
| ATOM | 1957 | CZ | PHE A 2 | 46 | 30. | 640 | 18.103 | 68.889 | 1.00 40.8 | 3 6 |
| | 1958 | Ċ | PHE A 2 | 46 | 27. | 970 | 19.311 | 73.371 | | |
| ATOM | | | PHE A 2 | 46 | 27. | 613 | 20.478 | 73.549 | 1.00 40.3 | 2 8 |
| ATOM | 1959 | | | | | 141 | 18.839 | | 1.00 42.5 | 4 7 |
| MOTA | 1960 | N | GLU A 2 | | 23. | 130 | 19.695 | | 1.00 43.9 | 36 |
| MOTA | 1961 | CA | GLU A 2 | 47 | | 128 | | | | |
| ATOM | 1962 | CB | GLU A 2 | 47 | | 655 | 19.075 | | | 3 6 |
| | 1963 | CG | GLU A 2 | 47 | 29. | 763 | 19.243 | | | |
| ATOM | | | | 47 | 28. | 478 | 18.424 | 76.962 | | 2 6 |
| ATOM | 1964 | CD | | | | 645 | 18.644 | | 1.00 62.1 | 2 8 |
| ATOM | 1965 | | 1 GLU A 2 | 4 / | | | 17.557 | | | 3 8 |
| ATOM | 1966 | OE. | 2 GLU A 2 | 47 | | .296 | | | | |
| | 1967 | | GLU A 2 | 47 | 31. | . 268 | 19.839 | | | |
| ATOM | | | GLU A 2 | 47 | 32. | .077 | 18.931 | 73.294 | 1.00 44.2 | |
| MOTA | 1968 | | | | | .342 | 20.988 | 72.780 | 1.00 43.6 | 5 7 |
| ATOM | 1969 | N | PRO A 2 | 40 | | | 22.143 | | | 3 6 |
| ATOM | 1970 | CD | | | | .439 | | | | |
| | 1971 | | PRO A 2 | 48 | | .371 | 21.260 | | | |
| ATOM | | | | 48 | 31 | .802 | 22.480 | | 1.00 43.0 | |
| ATOM | 1972 | | | 48 | | .317 | 22.474 | | 1.00 43.0 | 2 6 |
| ATOM | 1973 | | | | | .759 | 21.552 | | L 1.00 43.3 | 7 6 |
| ATOM | 1974 | C | PRO A 2 | 48 | | | | | 4- 4 | |
| ATOM | 1975 | | PRO A 2 | 48 | | .896 | 22.286 | | | |
| | 1976 | | GLU A 2 | 49 | 34 | .788 | 20.982 | | | |
| ATOM | | | | 49 | | .151 | 21.26 | 3 72.136 | | |
| ATOM | 1977 | | 010 A 2 | 140 | | .148 | 20.27 | | 1.00 42.0 | |
| ATOM | 1978 | | GLU A 2 | 4.7 | | | | | | 28 6 |
| ATOM | 1979 |) CG | GLU A 2 | 49 | 36 | .935 | 18.81 | - | | |
| | | | GLU A 2 | 249 | 38 | .015 | 17.90 | D /1.49 | , <u></u> . | - |
| ATOM | 1701 | | | | | | | - | • | |
| .* " | | | | • | | | | | | |
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|-------|-------|---|--------|--------|----------|------------|---|
| | | OE1 GLU A 249 | 38.208 | 17.938 | 70.054 | 1.00 42.47 | 8 |
| ATOM | 1981 | OET GEO H 243 | | 17.168 | 72.072 - | 1.00 39.73 | 8 |
| MOTA | 1982 | OE2 GLU A 249 | 38.666 | | | | 6 |
| | | C GLU A 249 | 36.443 | 22.654 | 71.583 | 1.00 40.99 | |
| MOTA | 1983 | | 37.150 | 23.450 | 72.204 | 1.00 42.83 | 8 |
| ATOM | 1984 | O GLU A 249 | | | | 1.00 37.65 | 7 |
| | 1985 | N VAL A 250 | 35.879 | 22.936 | 70.407 | | |
| MOTA | | N VIII 1 250 | 36.059 | 24.221 | 69.728 | 1.00 34.87 | 6 |
| ATOM | 1986 | CA VAL A 250 | - | | | 1.00 34.53 | 6 |
| | 1987 | CB VAL A 250 | 37.294 | 24.203 | 68.789 | | |
| ATOM | | CB VALUE 11 000 | 37.129 | 23.113 | 67.728 | 1.00 32.76 | 5 |
| MOTA | 1988 | CG1 VAL A 250 | | | - | 1.00 29.62 | 6 |
| | 1989 | CG2 VAL A 250 | 37.487 | 25.581 | 68.144 | | |
| MOTA | | | 34.830 | 24.527 | 68.891 | 1.00 32.67 | 6 |
| ATOM | 1990 | | | | 68.421 | 1.00 33.96 | 8 |
| ATOM | 1991 | O VAL A 250 | 34.162 | 23.610 | | | |
| | | 0.51 | 34.539 | 25.810 | 68.690 | 1.00 29.71 | 7 |
| MOTA | 1992 | N TYR A 251 | | 26.183 | 67.916 | 1.00 27.07 | 6 |
| ATOM | 1993 | CA TYR A 251 | 33.368 | | | | 6 |
| | 1994 | CB TYR A 251 | 32.185 | 26.451 | 68.860 | 1.00 29.11 | |
| MOTA | | | 32.080 | 27.872 | 69.406 | 1.00 31.46 | 6 |
| MOTA | 1995 | CG TYR A 251 | 52.000 | | 68.622 | 1.00 31.14 | 6 |
| MOTA | 1996 | CD1 TYR A 251 | 31.553 | 28.903 | | | |
| | | | 31.439 | 30.196 | 69.106 | 1.00 31.66 | 6 |
| MOTA | 1997 | | | 28.181 | 70.696 | 1.00 30.20 | 6 |
| MOTA | 1998 | CD2 TYR A 251 | 32.494 | | | | 6 |
| | | CE2 TYR A 251 | 32.384 | 29.477 | 71.193 | 1.00 33.89 | |
| ATOM | 1999 | | 31.854 | 30.482 | 70.391 | 1.00 34.75 | 6 |
| MOTA | 2000 | CZ TYR A 251 | | | 70.867 | 1.00 33.52 | 8 |
| ATOM | 2001 | OH TYR A 251 | 31.743 | 31.773 | | | 6 |
| | | | 33.570 | 27.384 | 66.992 | 1.00 27.48 | |
| MOTA | 2002 | C TYR A 251 | | 28.402 | 67.366 | 1.00 24.78 | 3 |
| ATOM | 2003 | O TYR A 251 | 34.167 | | | 1.00 24.80 | 7 |
| | 2004 | N LEU A 252 | 33.063 | 27.254 | 65.773 | | |
| MOTA | | | 33.150 | 28.332 | 64.815 | 1.00 23.40 | 6 |
| ATOM | 2005 | CA LEU A 252 | | | 63.451 | 1.00 21.32 | 6 |
| ATOM | 2006 | CB LEU A 252 | 33.631 | 27.810 | | | 6 |
| | | CG LEU A 252 | 35.126 | 27.456 | 63.385 | 1.00 21.84 | |
| ATOM | 2007 | | 35.457 | 26.373 | 64.395 | 1.00 22.51 | 6 |
| ATOM | 2008 | CD1 LEU A 252 | | | | 1.00 22.07 | 5 |
| | 2009 | CD2 LEU A 252 | 35.499 | 26.999 | 61.986 | | |
| MOTA | | | 31.762 | 28.959 | 64.729 | 1.00 22.56 | 6 |
| MOTA | 2010 | C LEU A 252 | | 28.266 | 64.856 | 1.00 21.99 | 8 |
| MOTA | 2011 | O LEU A 252 | 30.750 | | | 1.00 21.01 | 7 |
| | 2012 | N LEU A 253 | 31.734 | 30.277 | 64.554 | | 6 |
| MOTA | | | 30.498 | 31.047 | 64.461 | 1.00 18.89 | |
| MOTA | 2013 | 0 - 0 | | 31.944 | 65.695 | 1.00 20.05 | 6 |
| ATOM | 2014 | CB LEU A 253 | 30.352 | | | 1.00 21.61 | 6 |
| | 2015 | CG LEU A 253 | 29.198 | 32.942 | 65.842 | | |
| ATOM | | CD1 LEU A 253 | 27.849 | 32.220 | 65.860 | 1.00 22.23 | 6 |
| ATOM | 2016 | CDI LEO A 255 | 29.395 | 33.716 | 67.145 | 1.00 22.90 | 6 |
| MOTA | 2017 | CD2 LEU A 253 | | | 63.198 | 1.00 20.05 | 6 |
| MOTA | 2018 | C LEU A 253 | 30.539 | 31.901 | | | 8 |
| | | O LEU A 253 | 31.466 | 32.691 | 62.987 | 1.00 18.17 | |
| MOTA | 2019 | U EEO A 255 | 29.544 | 31.720 | 62.340 | 1.00 19.40 | 7 |
| ATOM | 2020 | N GLN A 254 | | | 61.115 | 1.00 18.17 | 6 |
| MOTA | 2021 | CA GLN A 254 | 29.488 | 32.490 | 01.113 | | 5 |
| | 2022 | CB GLN A 254 | 29.017 | 31.592 | 59.969 | | |
| MOTA | _ | | 27.584 | 31.713 | 59.601 | 1.00 18.43 | 6 |
| MOTA | 2023 | CG GLN A 254 | | | 58.549 | 1.00 19.97 | 6 |
| MOTA | 2024 | CD GLN A 254 | 27.368 | 32.766 | | 1.00 22.54 | 8 |
| | 2025 | OE1 GLN A 254 | 27.917 | 32.677 | 57.450 | 1.00 22.34 | |
| MOTA | | | 26.564 | 33.769 | 58.869 | 1.00 22.89 | 7 |
| MOTA | 2026 | NE2 GLN A 254 | | | 61.444 | 1.00 19.75 | 6 |
| MOTA | 2027 | C GLN A 254 | 28.520 | 33.634 | 01.444 | 1 00 19 77 | 8 |
| | | | 27.470 | 33.415 | 62.060 | 1.00 18.77 | |
| MOTA | 2028 | O GLN A 254 | | 34.854 | 61.067 | 1.00 23.02 | 7 |
| MOTA | 2029 | N LEU A 255 | 28.905 | | | 1.00 23.77 | 6 |
| | 2030 | CA LEU A 255 | 28.132 | 36.052 | 61.369 | | |
| MOTA | | CA DEC 11 2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 | 28.963 | 36.993 | 62.242 | 1.00 26.84 | 6 |
| ATOM | 2031 | CB LEU A 255 | | | 63.684 | 1.00 29.34 | 6 |
| ATOM | 2032 | CG LEU A 255 | 29.226 | 36.556 | | 1 00 30 65 | 6 |
| | | CD1 LEU A 255 | 30.196 | 37.520 | 64.331 | 1.00 30.65 | 9 |
| MOTA | 2033 | | 27.902 | 36.506 | 64.456 | 1.00 28.42 | 6 |
| ATOM | 2034 | CD2 LEU A 255 | | | 60.197 | 1.00 24.84 | 6 |
| | 2035 | C LEU A 255 | 27.605 | 36.842 | | 1 00 24 04 | 8 |
| MOTA | | 255 | 27.774 | 38.066 | 60.149 | 1.00 24.94 | - |
| MOTA | 2036 | O LEU A 255 | | 36.158 | 59.254 | 1.00 25.07 | 7 |
| ATOM | 2037 | N GLY A 256 | 26.969 | | | | 6 |
| | 2038 | CA GLY A 256 | 26.408 | | 58.117 | | 6 |
| ATOM | | | 25.506 | 37.956 | 58.644 | 1.00 27.11 | |
| ATOM | 2039 | C GLY A 256 | | | 59.584 | 1.00 25.67 | 8 |
| ATOM | 2040 | O GLY A 256 | 24.742 | | | | 7 |
| | 1041 | | 25.599 | | | | 5 |
| ATOM | | | 24.757 | | 58.536 | 1.00 29.28 | |
| MOTA | 2042 | | | | | | ć |
| ATOM | 2043 | CB THR A 257 | 25.517 | 41.007 | | | 8 |
| | 2044 | | 26.002 | | | | 6 |
| atom | | | 26.686 | | | 1.00 26.45 | |
| ATOM | 2045 | | | | | | 6 |
| 3 TOM | 10046 | C THR A 257 | 23.477 | 40.394 | | . = : | |

| | 2047 | _ | THR A | 257 | 22.747 | 41 | .370 | 57.879 | 1.00 29.49 | 8 |
|------|------|-----|-------|-------|-----------------|-----|------------------|------------------|--------------------------|--------|
| MOTA | 2047 | 0 ' | ASP A | 258 | 23.192 | | .414 | 56.867 | 1.00 29.13 | 7 |
| MOTA | 2048 | N . | AGP A | 250 | 21.977 | | .471 | 56.065 | 1.00 30.49 | 6 |
| MOTA | 2049 | | ASP A | | 22.004 | | 3.432 | 54.933 | 1.00 28.22 | 6 |
| MOTA | 2050 | | ASP A | | _ | | 7.033 | 55.416 | 1.00 29.39 | 6 |
| MOTA | 2051 | | ASP A | | 22.337 | | 5.653 | 56.520 | 1.00 30.16 | 8 |
| MOTA | 2052 | OD1 | ASP A | 258 | 21.893 | | | 54.667 | 1.00 29.97 | 8 |
| ATOM | 2053 | OD2 | ASP A | 258 | 23.019 | | 5.292 | | 1.00 30.50 | 6 |
| ATOM | 2054 | | ASP A | | 20.646 | | 3.355 | 56.826 | 1.00 30.30 | 8 |
| ATOM | 2055 | 0 | ASP A | 258 | 19.601 | | 622 | 56.248 | 1.00 32.87 | 7 |
| ATOM | 2056 | N | PRO A | 259 | 20.650 | | 3.912 | 58.101 | | 6 |
| ATOM | 2057 | CD | PRO A | 259 - | 21.713 | | 3.338 | 58.952 | 1.00 33.56 | 6 |
| MOTA | 2058 | CA | PRO A | 259 | 19.366 | | 3.821 | 58.806 | 1.00 31.73 | 6 |
| ATOM | 2059 | | PRO A | | 19.705 | | 7.912 | 59.987 | 1.00 31.87 | |
| ATOM | 2060 | CG | PRO A | 259 | 21.067 | | 3.373 | 60.333 | 1.00 31.73 | 6 |
| ATOM | 2061 | C | PRO A | 259 | 18.817 | | 0.184 | 59.260 | 1.00 30.86 | 6 |
| MOTA | 2062 | | PRO A | | 17.736 | | 0.270 | 59.845 | 1.00 29.78 | 8 . |
| ATOM | 2063 | | LEU A | | 19.56 | | 1.245 | 58.980 | 1.00 29.58 | 7 |
| MOTA | 2064 | | LEU A | | 19.16 | | 2.592 | 59.375 | 1.00 29.15 | 6 |
| ATOM | 2065 | | LEU A | | 20.36 | | 3.542 | 59.275 | 1.00 27.14 | 6 |
| ATOM | 2066 | | LEU A | | 21.54 | | 3.286 | 60.234 | 1.00 22.17 | 6 |
| ATOM | 2067 | | LEU A | | 22.79 | | 3.919 | 59.684 | 1.00 15.79 | 6 |
| ATOM | 2068 | CD2 | LEU A | 260 | 21.21 | 1 4 | 3.793 | 61.633 | 1.00 16.25 | 6 |
| ATOM | 2069 | C | LEU A | 260 | 17.99 | 24 | 3.165 | 58.576 | 1.00 28.09 | 6 |
| ATOM | 2070 | Ö | LEU A | | 17.78 | 74 | 2.834 | 57.410 | 1.00 29.61 | 8 |
| ATOM | 2071 | N | LEU A | 261 | 17.23 | 7 4 | 4.044 | 59.223 | 1.00 29.29 | 7 |
| ATOM | 2072 | CA | LEU A | | 16.09 | 74 | 4.693 | 58.596 | 1.00 29.71 | 6 |
| ATOM | 2073 | CB | LEU A | 261 | 15.54 | 0 4 | 5.788 | 59.513 | 1.00 29.62 | 6 |
| MOTA | 2074 | CG | LEU A | 261 | 14.40 | 6 4 | 6.664 | 58.950 | 1.00 28.14 | 6 |
| ATOM | 2075 | | LEU A | 261 | 13.14 | 4 4 | 5.819 | 58.803 | 1.00 24.82 | 6 |
| ATOM | 2076 | | LEU A | | 14.13 | 94 | 7.859 | 59.882 | 1.00 25.45 | 6 |
| ATOM | 2077 | C | LEU A | | 16.46 | | 5.322 | 57.259 | 1.00 29.50 | 6 |
| ATOM | 2078 | Õ | LEU A | | 15.71 | | 5.198 | 56.295 | 1.00 31.67 | 8 |
| ATOM | 2079 | N | GLU A | | 17.60 | 3 4 | 5.998 | 57.201 | 1.00 31.54 | 7 |
| ATOM | 2080 | CA | GLU A | 262 . | 18.01 | | 6.664 | 55.973 | 1.00 31.93 | 6 |
| ATOM | 2081 | CB | GLU A | | 19:04 | | 7.758 | 56.279 | 1.00 29.34 | 6 6 |
| ATOM | 2082 | CG | GLU A | 262 | 18.49 | | 8.931 | 57.086 | 1.00 28.52 1.00 29.76 | 6 |
| ATOM | 2083 | CD | GLU A | | 18.44 | - | 8.687 | 58.589 | | 8 |
| ATOM | 2084 | OE1 | GLU A | 262 | 18.17 | | 7.548 | 59.029 | 1.00 30.12 | 8 |
| ATOM | 2085 | OE2 | GLU A | 262 | 18.66 | | 9.661 | 59.338 | 1.00 27.05 | 6 |
| MOTA | 2086 | С | GLU A | 262 | 18.52 | _ | 5.754 | 54.857 53.722 | 1.00 35.20 | |
| MOTA | 2087 | 0 | GLU A | 262 | 18.69 | | 6.199 | 55.158 | 1.00 36.55 | |
| ATOM | 2088 | Ħ | ASP A | | 18.77 | 8 4 | 4.486 | 54.117 | 1.00 39.50 | |
| ATOM | 2089 | CA | ASP A | | 19.24 | | 3.582 | 54.641 | 1.00 38.42 | |
| ATOM | 2090 | CB | ASP A | 263 | 20.35 | - | 12.672 | 53.538 | 1.00 39.33 | |
| MOTA | 2091 | CG | ASP A | 263 | 20.98 | | 1.263 | 53.762 | 1.00 38.86 | |
| ATOM | 2092 | OD1 | ASP A | 263 | 22·.06 20.38 | | 1.779 | 52.443 | 1.00 39.50 | 8 |
| MOTA | 2093 | | ASP A | 203 | 18.04 | | 2.775 | 53.634 | 1.00 42.83 | 6 |
| ATOM | 2094 | C | ASP A | | 17.47 | | 11.966 | 54.381 | 1.00 44.22 | |
| MOTA | 2095 | 0 | ASP A | | 17.67 | | 13.002 | 52.377 | 1.00 44.14 | |
| MOTA | 2096 | N | TYR A | | 16.50 | - | 12.357 | 51.796 | 1.00 46.67 | 6 |
| MOTA | 2097 | CA | TYR A | | 16.03 | | 13.149 | 50.568 | 1.00 54.61 | . 6 |
| MOTA | 2098 | CB | TYR A | 264 | 16.82 | | 12.939 | 49.294 | 1.00 63.02 | |
| MOTA | 2099 | CG | TYR A | | 16.51 | | 11.897 | | 1.00 65.73 | |
| MOTA | 2100 | CD1 | | | 17.23 | | 11.709 | 47.226 | 1.00 68.35 | |
| MOTA | 2101 | CEI | | | 17.88 | | 43.786 | 48.962 | 1.00 66.23 | |
| MOTA | 2102 | CD2 | TYR A | | 18.61 | | 43.606 | 47.780 | 1.00 68.63 | |
| MOTA | 2103 | CE2 | | | | | 42.570 | 46.918 | 1.00 69.08 | 3 6 |
| ATOM | 2104 | CZ | TYR A | | 18.27 | | 42.411 | 45.746 | 1.00 69.01 | |
| MOTA | 2105 | OH | TYR A | | 18.98 | | 40.888 | 51.451 | 1.00 43.89 | 6 |
| MOTA | 2106 | Ç | TYR A | | 16.66 | | 40.885 40.185 | | 1.00 44.80 | 8 (|
| ATOM | 2107 | 0 | TYR A | | 15.66 | | 40.400 | | 1.00 40.3 | 7 |
| ATOM | 2108 | N | LEU A | | 17.89 | | 38.984 | | | 5 6 |
| ATOM | 2109 | CA | LEU A | | 18.05 19.4 | | 38.646 | | | 3 6 |
| ATCM | 2110 | CB | LEU A | | 19.4 | | 39.211 | | 1.00 32.43 | 36 |
| ATCM | 2111 | CG | LEU A | | 21.1 | | 38.535 | | | |
| ATOM | 2112 | CD1 | LEU A | 405 | ٠ | | J . J J J | | _ | |

| | | CD2 - | LEU A | 265 | 18 | .828 | 38.954 | 48.141 | 1.00 34.4 | |
|--------|------|--------|----------|---------|-----|--------|---------|----------|-----------|--------|
| ATOM | | | LEO A | 203 | | | 38.131 | 52.219 | 1.00 37.4 | 16. |
| MOTA | 2114 | C | LEU A | 265 | | .665 | | | | |
| | | 0 | LEU A | 265 | 18 | .125 | 37.000 | 52.370 | 1.00 37.9 | |
| MOTA | 2115 | | | | | .804 | 38.694 | 53.066 | 1.00 36.2 | 1 7 |
| ATOM | 2116 | | SER A | | | | | | 1.00 36.4 | |
| | 2117 | CA | SER A | 266 | 16 | . 294 | 38.013 | 54.253 | | _ |
| MOTA | | | | | 17 | .263 | 38.136 | 55.427 | 1.00 37.2 | 2 6 |
| ATOM - | 2118 | | SER A | | | | | | 1.00 37.4 | |
| | 2119 | OG | SER A | 266 | 17 | .190 | 39.440 | 55.991 | 1.00 37.4 | |
| ATOM | _ | | | | 1 4 | .997 | 38.705 | 54.653 | 1.00 35.5 | 5 6 |
| ATOM | 2120 | | SER A | | | | | 54.568 | 1.00 37.0 | 9 8 |
| ATOM | 2121 | 0 | SER A | 266 | | .889 | 39.927 | | | - |
| - | | | LYS A | | 1 Δ | .018 | 37.928 | 55.093 | 1.00 34.3 | - |
| MOTA | 2122 | | | | | 750 | 38.493 | 55.532 | 1.00 36.1 | 3 6 |
| MOTA | 2123 | CA | LYS A | 267 | 12 | .750 | | | | |
| | | | LYS A | | 11 | .596 | 37.548 | 55.183 | 1.00 36.1 | |
| MOTA | 2124 | | | | | .503 | 37.222 | 53.705- | 1.00 36.7 | 79 6 |
| ATOM | 2125 | | LYS A | | | | | 52.869 | 1.00 38.5 | |
| | 2126 | CD | LYS A | 267 | 11 | .453 | 38.487 | | | |
| MOTA | | CE | LYS A | 267 | 11 | 369 | 38.170 | 51.389 | 1.00 41.6 | 60 6 |
| ATOM | 2127 | CE | PI2 W | 207 | | | 39.413 | 50.569 | 1.00 42.0 |)7 7 - |
| ATOM | 2128 | NZ | LYS A | 267 | | 503 | | | | |
| | | С | LYS A | 267 | 12 | .791 | 38.738 | 57.043 | 1.00 34.9 | |
| MOTA | 2129 | | DID 7. | 207 | 11 | .758 | 38.867 | 57.694 | 1.00 37.3 | 18 8 |
| ATOM | 2130 | 0 | LYS A | 26/ | | | | | 1.00 32.8 | |
| | 2131 | N | PHE A | 268 | | .998 | 38.775 | 57.595 | 1.00 32.0 | |
| MOTA | | | PHE A | 268 | 1.4 | .192 | 39.021 | 59.016 | 1.00 31. | |
| ATOM | 2132 | CA | PRE A | 200 | | .477 | 38.337 | 59.495 | 1.00 34. | 05 6 |
| ATOM | 2133 | CB | PHE A | | | | | | 1.00 34. | 54 6 |
| | 2134 | CG | PHE A | 268 | 15 | 3.379 | 36.839 | 59.604 | | |
| ATOM | | | | | 1.6 | 5.506 | 36.087 | 59.940 | 1.00 35. | 04 6 |
| MOTA | 2135 | CD1 | | | | | | 59.429 | 1.00 34. | |
| ATOM | 2136 | CD2 | PHE A | . 268 · | 14 | 1.161 | 36.178 | | | |
| | | CEl | PHE A | 268 | 16 | 5.423 | 34.691 | 60.108 | 1.00 35. | |
| MOTA | 2137 | | | | | 1.066 | 34.784 | 59.594 | 1.00 36. | 00 6 |
| ATOM | 2138 | CE2 | PHE A | | | | | | 1.00 34. | |
| | 2139 | CZ | PHE A | 258 | 1: | 5.201 | 34.040 | 59.936 | | |
| MOTA | | | PHE A | | 14 | 4.319 | 40.530 | 59.190 | 1.00 30. | |
| MOTA | 2140 | С | PRE A | 200 | | | 41.192 | 58.394 | 1.00 30. | 27 8 |
| MOTA | 2141 | 0 | PHE A | 268 | | 4.983 | | | | - |
| | 2142 | N | ASN A | 269 | 13 | 3.693 | 41.081 | 60.222 | | |
| ATOM | | | | | · 1 | 3.760 | 42.527 | 60.448 | 1.00 35. | 83 6 |
| ATOM | 2143 | CA | ASN A | 209 | | | | 60.570 | 1.00 37. | 23 6 |
| MOTA | 2144 | CB | ASN A | 269 | | 2.344 | 43.115 | | 1 00 40 | |
| | | CG | ASN A | 269 | 1: | 1.478 | 42.809 | 59.360 | 1.00 40. | |
| MOTA | 2145 | | 3.531 | 260 | 3 . | 1.830 | 43.148 | 58.227 | 1.00 43. | |
| ATOM | 2146 | OD1 | ASN A | 1 209 | | | | 59.594 | 1.00 39. | 61 7 |
| MOTA | 2147 | ND2 | ASN A | A 269 | | 0.335 | 42.165 | | 1.00 35. | |
| | 2148 | С | ASN A | 269 | 1 | 4.553 | 42.854 | 61.710 | 1.00 33. | |
| ATOM | | | ASN A | 360 | 1 | 4.095 | 43.621 | 62.560 | 1.00 41. | 47 8 |
| ATOM | 2149 | 0 | ASN A | 4 209 | | | 42.285 | 61.827 | 1.00 33. | 27 7 |
| MOTA | 2150 | N | LEU A | ¥ 270 | | 5.747 | | | 1.00 30. | |
| | 2151 | CA | LEU A | A 270 | | 6.571 | 42.510 | 63.004 | | |
| MOTA | | | LEU A | 270 | 1 | 7.638 | 41.431 | 63.114 | 1.00 27. | |
| MOTA | 2152 | CB | LEU A | 270 | | 7.140 | | 62.988 | 1.00 23. | .76 6 |
| ATOM | 2153 | CG | LEU A | A 270 | | | | | 1.00 27. | |
| ATOM | 2154 | CD1 | LEU A | A 270 | 1 | 8.222 | | | | |
| | | | | 270 | 1 | 5.855 | 39.801 | 63.772 | 1.00 28. | |
| ATOM | 2155 | CD2 | LEU A | 270 | | 7.258 | | 63.Q33 | 1.00 32 | .30 6 |
| MOTA | 2156 | С | LEU A | A 270 | | | | | 1.00 36 | .27 8 |
| | 2157 | 0 | LEU | A 270 | 1 | 7.347 | 44.554 | | 1.00 30 | |
| MOTA | | | CEB | A 271 | 1 | 7.749 | 44.207 | 64.216 | 1.00 30 | |
| MOTA | 2158 | N | 3EK 1 | | | 8.465 | | 64.424 | 1.00 30 | .79 6 |
| ATOM | 2159 | CA | SER A | A 271 | | | | | 1.00 29 | .53 6 |
| ATOM | 2160 | CB | SER A | A 271 | 1 | 7.816 | | | | . 43 |
| | | | CEP | A 271 | . 1 | 7.712 | 45.471 | 66.739 | 1.00 30 | .43 8 |
| ATOM | 2161 | OG | SER A | - 051 | | | | | 1.00 33 | .09 6 |
| MOTA | 2162 | С | SER A | A 271 | | 9.911 | | | | |
| | 2163 | 0 | SER | a 271 | 2 | 0.194 | 43.972 | | | |
| MOTA | | | 3 CM | A 272 | 2 | 0.821 | 46.069 | 64.586 | 1.00 32 | .36 7 |
| ATOM | 2164 | N | ASN . | A 2/2 | | | | | | .65 6 |
| MOTA | 2165 | CA | ASN . | A 272 | | 2.234 | | | | |
| | 2166 | CB | 2 SN | A 272 | 2 | 23.036 | 47.141 | | | |
| ATOM | | | | | 7 | 3.101 | 47.658 | 63.361 | 1.00 37 | .76 6 |
| ATOM | 2167 | CG | ASN | A 272 | | | | · | | .12 8 |
| ATOM | 2168 | OD1 | ASN | A 272 | | 23.719 | | | | |
| | 2169 | 2 מונו | NZA | A 272 | 2 | 22.460 | 46.952 | | | |
| ATOM | | | | 272 | | 22.369 | | 66.321 | 1.00 32 | |
| ATOM | 2170 | С | | A 272 | | | | | | .95 8 |
| ATOM | 2171 | 0 | ASN | A 272 | | 22.970 | | | | |
| | | N | VAT. | A 273 | 2 | 21.803 | 46.09 | | | |
| MOTA | 2172 | | **** | 272 | | 21.839 | | 1 68.668 | 1.00 35 | .52 6 |
| ATOM | 2173 | CA | VAL | A 273 | | | | | | .80 6 |
| ATCM | 2174 | CB | VAL | A 273 | | 20.92 | | | | |
| | | CG1 | L VAL | a 273 | - : | 20.98 | 7 46.27 | | | .00 |
| ATCM | 2175 | ~~ | | 3 273 | | 21.35 | 6 48.11 | 2 69.275 | 1.00 38 | |
| ATOM | 2176 | | 2 VAL | M 213 | | | | | | .26 6 |
| ATCM | 2177 | С | VAL | A 273 | | 21.41 | | | | |
| | | | TAL | A 273 | | 22.06 | 0 43.58 | 0 69.679 | 1.00 33 | ,.,, |
| 2.TCM | 2178 | 9 | ۷ | | | _ | | - | | |

| | | | | _ | | | 42 000 | 68.262 | 1.00 32 | 2 3 6 | 7 |
|--------|------|------|-------------|-----|-----|--------|--------|--------|---------|-------|-----|
| 3.0004 | 2179 | N | ALA A 274 | - 2 | 20. | .328 | 43.889 | | | | |
| ATCM | | | ALA A 274 | | 19 | . 834 | 42.521 | 68.385 | 1.00 3 | | 6 |
| ATCM | 2180 | CA | | | | .574 | 42.356 | 67.578 | 1.00 2 | 8.88 | 6 |
| ATCM | 2181 | CB | ALA A 274 | | | | | 67.861 | 1.00 3 | | 6 |
| ATCM | 2182 | С | ALA A 274 | | | .923 | 41.588 | | | | 8 |
| | | ō | ALA A 274 | | 21 | .323 | 40.634 | 68.533 | 1.00 3 | | |
| MOTA | 2183 | | 275 | | | .401 | 41.879 | 66.655 | 1.00 3 | 0.05 | 7 |
| ATCM | 2184 | N | PHE A 275 | | | | 41.102 | 66.036 | 1.00 3 | 1.30 | 6 |
| ATCM | 2185 | CA | PHE A 275 | | | .467 | | | 1.00 3 | | 6 |
| | 2186 | CB | PHE A 275 | | 22 | .932 | 41.810 | 64.751 | | | |
| ATCM | | | PHE A 275 | | 23 | .938 | 41.029 | 63.941 | 1.00 3 | 1.76 | 6 |
| ATCM | 2187 | CG | PRE A 275 | | | .597 | 39.809 | 63.365 | 1.00 3 | 2.40 | 6 |
| ATCM | 2188 | CD1 | PHE A 275 | | | | | 63.729 | 1.00 3 | 4.04 | 6 |
| ATCM | 2189 | CD2 | PHE A 275 | | | .219 | 41.529 | | 1.00 3 | 2.02 | 6 |
| | 2190 | CEI | PHE A 275 | | 24 | .513 | 39.100 | 62.586 | 1.00 3 | | |
| MCTA | | | PHE A 275 | | | .149 | 40.828 | 62.950 | 1.00 3 | | 6 |
| MOTA | 2191 | CE2 | | | | .793 | 39.613 | 62.378 | 1.00 3 | 4.50 | 6 |
| MCTA | 2192 | cz | PHE A 275 | | | | | 67.040 | 1.00 2 | 9 98 | 6 |
| MOTA | 2193 | С | PHE A 275 | | | .632 | 40.999 | | 1.00 2 | | 8 |
| | 2194 | Ö | PHE A 275 | | 24 | .252 | 39.950 | 67.200 | 1.00 2 | 9.41 | |
| ATCM | | | LEU A 276 | | 23 | .908 | 42.099 | 67.726 | 1.00 3 | 1.22 | 7 |
| MOTA | 2195 | N | LEU A 270 | | | .988 | 42.144 | 68.698 | 1.00 3 | 2.29 | 6 |
| ATCM | 2196 | CA | LEU A 276 | | | | | 69.141 | 1.00 3 | 3.44 | 6 |
| ATCM | 2197 | CB | LEU A 276 | | | .221 | 43.594 | | 1.00 3 | 6 01 | 6 |
| | 2198 | CG | LEU A 276 | | 26 | .415 | 43.908 | 70.050 | 1.00 3 | 0.01 | |
| ATOM | | | | | 26 | .683 | 45.391 | 70.025 | 1.00 3 | | 6 |
| ATCM | 2199 | CD1 | LEU A 270 | | | .147 | 43.433 | 71.467 | 1.00 3 | 39.09 | 6 |
| MOTA | 2200 | CD2 | LEU. A 276 | | | | | 69.894 | 1.00 3 | 32.79 | 6 |
| ATCM | 2201 | С | LEU A 276 | | | .682 | 41.244 | 09.094 | 1.00 3 | 0 74 | 8 |
| | 2202 | ŏ | LEU A 276 | | 25 | .560 | 40.530 | 70.371 | | | |
| ATOM | | | LYS A 277 | | 23 | .445 | 41.273 | 70.384 | 1.00 3 | 33.95 | 7 |
| ATCM | 2203 | N | DIS A 277 | | 22 | .086 | 40.413 | 71.505 | 1.00 | 36.56 | 6 |
| ATCM | 2204 | CA | LYS A 277 | | 23 | .000 | | 71.902 | 1.00 | | 6 |
| ATOM | 2205 | CB | LYS A 277 | | 21 | 623 | 40.588 | | 1.00 | | 6 |
| | 2206 | CG | LYS A 277 | | 21 | L.343 | 41.842 | 72.687 | 1.00 | 45.31 | |
| ATCM | | | LYS A 277 | | 20 | .743 | 41.508 | 74.049 | 1.00 | 45.72 | 6 |
| MOTA | 2207 | CD | LIS A 277 | | | 1.665 | 40.601 | 74.865 | 1.00 | 47.87 | 6 |
| ATOM | 2208 | CĒ | LYS A 277 | | | | 40.378 | 76.244 | 1.00 | 44.36 | 7 |
| ATCM | 2209 | NZ | LYS A 277 | | | L.140 | | | 1.00 | | 6 |
| | 2210 | C | LYS A 277 | | 23 | 3.302 | 38.974 | 71.092 | 1.00 | 37.30 | |
| MCTA | | | LYS A 277 | | | 3.875 | 38.179 | 71.845 | 1.00 | 37.54 | 8 |
| MOTA | 2211 | 0 | | | | 2.832 | 38.654 | 69.886 | 1.00 | 37.17 | 7 |
| ATOM | 2212 | N | ALA A 278 | | | | 37.311 | 69.323 | 1.00 | 34.51 | 6 |
| ATOM | 2213 | CA | ALA A 278 | | | 2.952 | | | 1.00 | 35 38 | 6 |
| | 2214 | CB | ALA A 278 | | | 2.638 | 37.341 | 67.820 | 1.00 | 33.30 | 6 |
| MCTA | | | ALA A 278 | | 24 | 4.368 | 36.831 | 69.550 | 1.00 | 30.63 | |
| ATOM | 2215 | C | ALA A 270 | | | 4.605 | 35.790 | 70.167 | 1.00 | 27.62 | 8 |
| ATOM | 2216 | 0 | ALA A 278 | | | | 37.624 | 69.049 | 1.00 | 29.24 | 7 |
| ATOM | 2217 | N | PHE A 279 | | | 5.303 | | 69.167 | 1 00 | 31.48 | 6 |
| | 2218 | CA | PHE A 279 | | | 6.722 | 37.347 | | | | 6 |
| ATCM | | CB | PHE A 279 | | 2 | 7.490 | 38.558 | 68.645 | | 33.25 | |
| ATOM | 2219 | | PHE A 279 | | | 8.974 | 38.396 | 68.663 | 1.00 | 39.28 | 6 |
| ATOM | 2220 | CG | PHE A 2/3 | | | 9.578 | 37.337 | 68.000 | 1.00 | 41.15 | 6 |
| ATOM | 2221 | CD: | 1 PHE A 279 | | | | | | | 40.66 | 6 |
| ATOM | 2222 | CD: | 2 PHE A 279 | | 2 | 9.776 | 39.328 | | | 44.22 | 6 |
| | 2223 | CE | 1 PHE A 279 | | 3 | 0.960 | 37.209 | 67.987 | | 44.22 | |
| ATOM | | CD. | 2 DUE 3 279 | | ٦ | 1.153 | 39.213 | 69.378 | 1.00 | 41.38 | 6 |
| ATOM | 2224 | | 2 PHE A 279 | | | 1.750 | 38.152 | | | 44.52 | 6 |
| ATOM | 2225 | CZ | PHE A 279 | | | | | | | 31.81 | 6 |
| ATCM | 2226 | С | PHE A 279 | | _ | 7.116 | 37.043 | | | 27.51 | 8 |
| A.C.M | 2227 | Ō | PHE A 279 | | 2 | 7.627 | 35.953 | 70.935 | | 27.31 | |
| ATOM | | | ASN A 280 | | | 6.860 | | 71.503 | 1.00 | 29.32 | 7 |
| ATOM | 2228 | N | ASN A 260 | | | 7.192 | | | | 29.26 | 6 |
| ATOM | 2229 | CA | | | | | | | | 30.39 | 6 |
| | 2230 | CB | ASN A 280 | | 2 | 6.927 | 39.153 | | | 30.50 | 6 |
| ATOM | | | | | 2 | 7.907 | 40.245 | 73.278 | 1.00 | 30.68 | 0 |
| ATOM | 2231 | | ASN A 200 | | | 9.117 | | | 1.00 | 33.34 | 8 |
| ATOM | 2232 | OD | 1 ASN A 280 | | | | _ | | | 27.00 | 7 |
| ATOM | 2233 | ND | 2 ASN A 280 | | | 7.395 | | | | 30.01 | 6 |
| | 2234 | | ASN A 280 | | | 6.524 | | | | 20 50 | 8 |
| ATCM | | | ASN A 280 | | | 7.167 | | 74.419 | | 29.58 | |
| ATOM | 2235 | | A3N A 200 | | | 5.252 | | | 1.00 | 30.46 | 7 |
| ATOM | 2236 | N | ILE A 281 | | | | | | | 33.71 | 6 |
| ATOM | 2237 | CA | ILE A 281 | | | 4.594 | | | | 36.14 | |
| | | | | | 2 | 23.107 | 35.16 | | | 26 10 | |
| ATOM | 2238 | | | | | 22.541 | | 74.032 | | 36.18 | |
| ATOM | 2239 | | 2 1LE M 201 | | | 22.298 | | 74.17 | 7 1.00 | 33.52 | 6 |
| ATCM | 2240 |) CG | 1 ILE A 281 | | : | 20.035 | 26.30 | | | 37.16 | 6 |
| | | | 1 ILE A 281 | | | 20.835 | | _ | | 34.06 | |
| ATCM | | | ILE A 281 | | - 2 | 25.330 | 34.00 | | | 21 04 | |
| ATOM | 2242 | | ILE A 281 | | • | 25.385 | 33.07 | | | 31.94 | |
| ATOM | 2243 | | | | | 25.896 | | | 7 1.00 | 35.31 | . 7 |
| | 2244 | ı N | VAL A 282 | | | ٠,٠٠٧ | | | | | |

| | | | | | | | | 1 00 36 45 | 6 |
|--------|------|-----|-------------|---|--------|--------|----------|--------------------------|---|
| ATOM | 2245 | CA | VAL A 282 | | 26.654 | 32.785 | | 1.00 36.45 1.00 35.62 | 6 |
| ATOM | 2246 | CB | VAL A 282 | | 27.084 | 32.871 | 70.524 | | 6 |
| ATOM | 2247 | CG1 | VAL A 282 | | 27.829 | 31.604 | 70.126 | | 6 |
| ATOM | 2248 | CG2 | VAL A 282 | | 25.880 | 33.080 | 69.646 | 1.00 34.51 | 6 |
| MOTA | 2249 | C | VAL A 282 | | 27.919 | 32.723 | 72.857 | 1.00 37.80 | 8 |
| | 2250 | ō | VAL A 282. | | 28.182 | 31.722 | 73.532 | 1.00 36.12 | 7 |
| MOTA | | N | ARG A 283 | | 28.693 | 33.808 | 72.821 | 1.00 38.45 | |
| MOTA | 2251 | CA | ARG A 283 | | 29.929 | 33.884 | 73.587 | 1.00 40.06 | 6 |
| MOTA | 2252 | | ARG A 283 | | 30.551 | 35.272 | 73.449 | 1.00 39.38 | 6 |
| MOTA | 2253 | CB | ARG A 283 | | 30.974 | 35.625 | 72.027 | 1.00 41.90 | 6 |
| MOTA | 2254 | CG | ARG A 283 | • | 31.492 | 37.048 | 71.968 | 1.00 41.36 | 6 |
| MOTA | 2255 | CD | ARG A 283 | | 32.647 | 37.206 | 72.840 | 1.00 43.35 | 7 |
| MOTA | 2256 | NE | ARG A 283 | | 33.162 | 38.373 | 73.215 | 1.00 42.55 | 6 |
| ATOM | 2257 | CZ | ARG A 283 | | 32.628 | 39.516 | 72.797 | 1.00 39.95 | 7 |
| ATOM | 2258 | NH1 | ARG A 283 | | 34.220 | 38.392 | 74.014 | 1.00 41.72 | 7 |
| ATOM | 2259 | NH2 | ARG A 283 | | 29.614 | 33.587 | 75.044 | 1.00 40.01 | 6 |
| MOTA | 2260 | C | ARG A 283 | | 30.350 | 32.862 | 75.716 | 1.00 39.01 | 8 |
| ATOM | 2261 | 0 | GLU A 284 | | 28.506 | 34.141 | 75.520 | 1.00 40.30 | 7 |
| MOTA | 2262 | N | GLU A 284 | | 28.084 | 33.923 | 76.894 | 1.00 43.19 | 6 |
| MOTA | 2263 | CA | GLU A 284 | | 26.753 | 34.647 | 77.165 | 1.00 47.53 | 6 |
| MOTA | 2264 | CB | | | 26.875 | 36.176 | 77.090 | 1.00 56.10 | 6 |
| MOTA | 2265 | CG | GLU A 284 | | 25.542 | 36.923 | 77.179 | 1.00 60.77 | 6 |
| MOTA | 2266 | CD | GLU A 284 | | 24.659 | 36.682 | 76.329 | 1.00 61.41 | 8 |
| ATOM | 2267 | OE1 | GLU A 284 | | 25.383 | 37.763 | 78.096 | 1.00 62.21 | 8 |
| MOTA | 2268 | OE2 | | | 27.953 | 32.429 | 77.179 | 1.00 40.72 | 6 |
| ATOM | 2269 | С | GLU A 284 | | 28.565 | 31.922 | 78.120 | 1.00 45.29 | 8 |
| MOTA | 2270 | 0 | GLU A 284 | | 27.186 | 31.721 | 76.354 | 1.00 34.82 | 7 |
| MOTA | 2271 | N | VAL A 285 | | 26.975 | 30.288 | 76.551 | 1.00 30.84 | 6 |
| MOTA | 2272 | CA | VAL A 285 | • | 25.842 | 29.752 | 75.647 | 1.00 27.74 | 6 |
| ATOM | 2273 | CB | VAL A 285 | | 25.698 | 28.253 | 75.831 | 1.00 22.95 | 6 |
| MOTA | 2274 | CG1 | VAL A 285 | | 24.545 | 30.433 | 75.982 | 1.00 26.26 | 6 |
| ATOM | 2275 | | VAL A 285 | | | 29.366 | 76.341 | 1.00 31.93 | 6 |
| MOTA | 2276 | С | VAL A 285 | | 28.181 | 28.556 | 77.214 | 1.00 33.46 | 8 |
| MOTA | 2277 | 0 | VAL A 285 | | 28.492 | 29.336 | 75.191 | 1.00 29.43 | 7 |
| MOTA | 2278 | N | PHE A 286 | | 28.845 | 28.586 | 74.907 | 1.00 24.26 | 6 |
| MOTA | 2279 | CA | PHE A 286 | | 29.973 | 27.957 | 73.519 | 1.00 22.57 | 6 |
| ATOM | 2280 | CB | PHE A 286 | | 29.830 | 27.095 | 73.345 | 1.00 23.46 | 6 |
| ATOM | 2281 | CG | PHE A 286 | | 28.607 | 27.639 | 72.885 | 1.00 23.90 | 6 |
| MOTA | 2282 | CD1 | PHE A 286 | | 27.409 | 25.718 | 73.608 | 1.00 21.95 | 6 |
| ATOM | 2283 | CD2 | | | 28.664 | 26.814 | 72.681 | 1.00 24.90 | 6 |
| MOTA | 2284 | CE1 | PHE A 286 | | 26.281 | 24.892 | 73.411 | 1.00 18.06 | 6 |
| ATOM | 2285 | CE2 | 2 PHE A 286 | | 27.547 | 25.437 | 72.945 | 1.00 20.23 | 6 |
| ATOM | 2286 | CZ | PHE A 286 | | 26.357 | 29.200 | 74.991 | 1.00 25.14 | 6 |
| MOTA | 2287 | С | PHE A 286 | | 31.368 | 28.566 | 74.560 | 1.00 23.16 | 8 |
| MOTA | 2288 | 0 | PHE A 286 | | 32.338 | 30.416 | 75.525 | 1.00 25.51 | 7 |
| MOTA | 2289 | N | GLY A 287 | | 31.480 | | 75.614 | 1.00 26.86 | 6 |
| MOTA | 229 | CA | GLY A 287 | | 32.783 | 31.511 | 74.270 | 1.00 26.28 | 6 |
| ATOM | 2291 | С | GLY A 287 | | 33.353 | 31.549 | 73.271 | 1.00 26.29 | 8 |
| MOTA | 2294 | 0 | GLY A 287 | | 32.644 | | 74.238 | 1.00 27.17 | 7 |
| ATOM | 2293 | N | GLU A 288 | | 34.637 | 31.849 | 72.996 | 1.00 33.20 | 6 |
| MOTA | 2294 | CA | GLU A 288 | | 35.274 | 32.291 | 73.269 | 1.00 35.09 | 6 |
| ATOM | 2295 | CB | GLU A 288 | | 36.680 | | 74.083 | 1.00 41.67 | 6 |
| ATOM | 2296 | CG | | | 36.726 | | 73.421 | 1.00 43.13 | 6 |
| ATOM | 2297 | CD | GLU A 288 | | 35.970 | | | | 8 |
| ATOM | 2298 | OE | 1 GLU A 288 | | 36.221 | 35.493 | | | 8 |
| MOTA | 2299 | | | | 35.130 | | | | 6 |
| ATOM | 2300 |) C | GLU A 288 | | 35.386 | | | | 8 |
| MOTA | 2301 | _ | GLU A 288 | | 35.596 | | | | 7 |
| ATOM | 2302 | | GLY A 289 | | 35.268 | 31.619 | | | 6 |
| MOTA | 2303 | | GLY A 289 | | 35.373 | | | | 6 |
| ATOM | 2304 | | GLY A 289 | | 35.948 | | | | 8 |
| ATOM | 2305 | | GLY A 289 | | 36.556 | | | | 7 |
| ATOM | 2306 | | VAL A 290 | | 35.764 | | | | 6 |
| ATOM | 2307 | | VAL A 290 | | 36.277 | | | | 6 |
| ATOM | 2308 | CB | VAL A 290 | | 37.014 | | | | 6 |
| · ATOM | 2309 | CG | 1 VAL A 290 | | 37.616 | | | | 6 |
| ATOM | | _ | 2 VAL A 290 | | 38.100 | 29.632 | , 05.832 | | |
| **** | | | | | | | | | |

| | | | | | | | | | _ |
|------|------|-------|-----------|---|--------|--------|---|------------|-----|
| • | | | AL A 290 | | 35.137 | 31.975 | 65.105 | 1.00 25.97 | 6 |
| ATOM | 2311 | | | | | | 64.672 | 1.00 22.32 | 8 |
| ATOM | 2312 | O 7. | AL A 290 | | 34.218 | | | 1.00 22.32 | 7 |
| | 2313 | | YR A 291 | | 35.217 | 33.293 | 64.914 | 1.00 27.33 | |
| MOTA | | 1/1 | 17 7 201 | | 34.188 | 34.052 | 64.203 | 1.00 26.69 | 6 |
| ATOM | 2314 | CA T | YR A 291 | | | | 64.939 | 1.00 25.51 | 6 |
| ATOM | 2315 | CB T | YR A 291 | | 33.925 | 35.356 | 54.333 | | |
| | | | YR A 291 | | 33.935 | 35.178 | 66.435 | 1.00 28.73 | 6 |
| MOTA | 2316 | CGT | IK A 221 | | | 35.596 | 67.191 | 1.00 29.72 | 6 |
| MOTA | 2317 | CD1 T | YR A 291 | | 35.025 | | | 1.00 29.53 | 6 |
| | 2318 | CE1 T | YR A 291 | | 35.059 | 35.414 | 68.563 | 1.00 25.33 | |
| MOTA | | | YR A 291 | | 32.874 | 34.565 | 67.094 | 1.00 27.39 | 6 |
| ATOM | 2319 | CD2 T | 1K A .291 | | 32.898 | 34.377 | 68.466 | 1.00 31.03 | 6 |
| MOTA | 2320 | | YR A 291 | | | 34.377 | | 1.00 31.85 | 6 |
| | 2321 | CZ T | YR A 291 | - | 33.997 | 34.808 | 69.194 | 1.00 31.03 | |
| MOTA | | | YR A 291 | | 34.030 | 34.647 | 70.562 | 1.00 38.03 | 8 . |
| ATOM | 2322 | | | | 34.527 | 34.345 | 62.745 | 1.00 27.99 | 6 |
| ATOM | 2323 | | YR A 291 | | | | 62.415 | 1.00 24.83 | 8 |
| ATOM | 2324 | O T | YR A 291 | | 35.608 | 34.843 | | 1.00 24.03 | 7 |
| | | _ | EU A 292 | | 33.567 | 34.042 | 61.880 | 1.00 30.17 | |
| MOTA | 2325 | | | | 33.726 | 34.220 | 60.441 | 1.00 28.26 | 6 |
| MOTA | 2326 | CA L | EU A 292 | | | | 59.741 | 1.00 27.70 | 6 |
| ATOM | 2327 | CB L | EU A 292 | | 33.561 | 32.861 | | 1.00 24.64 | 6 |
| | 2328 | CG L | LEU A 292 | | 34.191 | 31.643 | 60.435 | | |
| MOTA | | | x 202 | | 33.867 | 30.380 | 59.661 | 1.00 24.66 | 6 |
| ATOM | 2329 | CD1 L | EU A 292 | | | | 60.553 | 1.00 23.19 | 6 |
| ATOM | 2330 | CD2 L | LEU A 292 | | 35.686 | 31.825 | | 1.00 25.59 | 6 |
| | 2331 | C I | LEU A 292 | | 32.649 | 35.175 | 59.944 | | |
| MOTA | | - | LEU A 292 | | 31.640 | 35.394 | 60.611 | 1.00 18.11 | 8 |
| ATOM | 2332 | 0 I | JEU A 232 | | | 35.749 | 58.770 | 1.00 28.55 | 7 |
| MOTA | 2333 | N C | GLY A 293 | | 32.869 | | | 1.00 31.26 | 6 |
| | 2334 | CA C | GLY A 293 | | 31.878 | 36.653 | 58.223 | | |
| MOTA | | ~ ~ | JLY A 293 | | 30.722 | 35.815 | 57.714 | 1.00 34.84 | 6 |
| MOTA | 2335 | C C | 3LI A 200 | | 30.463 | 34.724 | 58.234 | 1.00 34.11 | 8 |
| MOTA | 2336 | 0 0 | GLY A 293 | | | | 56.689 | 1.00 35.34 | 7 |
| ATOM | 2337 | N C | GLY A 294 | | 30.036 | 36.312 | | | 6 |
| | | CA C | GLY A 294 | | 28.918 | 35.581 | 56.124 | 1.00 34.84 | |
| MOTA | 2338 | | | | 28.142 | 36.445 | 55.155 | 1.00 34.79 | 6 |
| ATOM | 2339 | C .(| GLY A 294 | | | 37.473 | 54.699 | 1.00 37.05 | 8 |
| MOTA | 2340 | 0 (| GLY A 294 | | 28.644 | | - | 1.00 31.87 | 7 |
| | 2341 | И | GLY A 295 | | 26.917 | 36.035 | 54.842 | | |
| MOTA | | | GLY A 295 | | 26.102 | 36.806 | 53.925 | 1.00 27.78 | 6 |
| MOTA | 2342 | CA (| GLI A 200 | | 25.969 | 38.245 | 54.378 | 1.00 27.09 | 6 |
| ATOM | 2343 | C (| GLY A 295 | | | | 55.546 | 1.00 27.03 | 8 |
| ATOM | 2344 | 0 (| GLY A 295 | | 26.192 | 38.558 | | 1.00 27.03 | 7 |
| | | N (| GLY A 296 | | 25.596 | 39.119 | 53.450 | 1.00 24.67 | |
| MOTA | 2345 | IN V | GD1 V 200 | | 25.440 | 40.527 | 53.7 57 | 1.00 25.28 | 6 |
| ATOM | 2346 | CA (| GLY A 296 | | | 41.262 | 52.446 | 1.00 27.64 | 6 |
| ATOM | 2347 | C | GLY A 296 | | 25.562 | | | 1.00 26.65 | 8 |
| | 2348 | 0 | GLY A 296 | | 26.591 | 41.163 | 51.771 | 1.00 20.03 | 7 |
| MOTA | | NI I | TYR A 297 | | 24.526 | 42.009 | 52.078 | 1.00 30.21 | |
| ATOM | 2349 | N | _IN N 207 | | 24.543 | 42.704 | 50.801 | 1.00 30.62 | 6 |
| ATOM | 2350 | CA | TYR A 297 | | _ | 42.011 | 49.859 | 1.00 29.50 | 6 |
| ATOM | 2351 | CB | TYR A 297 | | 23.560 | | 40.053 | 1.00 30.33 | 6 |
| | 2352 | CG | TYR A 297 | | 23.717 | 40.516 | 49.953 | 1.00 30.33 | |
| MOTA | | CD1 | TYR A 297 | | 23.174 | 39.810 | 51.031 | 1.00 30.86 | 6 |
| ATOM | 2353 | CD1 | A 207 | | 23.450 | 38.449 | 51.226 | 1.00 30.74 | 6 |
| ATOM | 2354 | CE1 | TYR A 297 | | | | 49.062 | 1.00 31.20 | 6 |
| ATOM | 2355 | CD2 | TYR A 297 | | 24.538 | 39.824 | | 1.00 32 08 | 6 |
| | 2356 | | TYR A 297 | | 24.821 | 38.460 | 49.247 | 1.00 32 00 | |
| MOTA | | | TYR A 297 | | 24.275 | 37.781 | 50.332 | 1.00 30 92 | 6 |
| MOTA | 2357 | CZ | 11K A 237 | | | 36.440 | 50.509 | 1.00 29 60 | 8 |
| MOTA | 2358 | OH | TYR A 297 | | 24.539 | | | 1.00 32.07 | 6 |
| ATOM | 2359 | С | TYR A 297 | | 24.267 | 44.195 | 50.875 | | 8 |
| | | ~ | TYR A 297 | | 24.134 | 44.849 | 49.840 | 1.00 33.83 | - |
| MOTA | 2360 | 0 | 11K H 201 | | 24.180 | 44.725 | 52.094 | 1.00 31.41 | 7 |
| MOTA | 2361 | N | HIS A 298 | | | | 52.289 | | 6 |
| ATOM | 2362 | CA | HIS A 298 | | 23.961 | 46.153 | | | 6 |
| | 2363 | CB | HIS A 298 | | 22.761 | 46.430 | 53.194 | | ~ |
| ATOM | | | HIS A 298 | | 22.379 | 47.880 | 53.256 | 1.00 35.16 | 6 |
| MOTA | 2364 | CG | 315 A 230 | | | 48.809 | | | 6 |
| MOTA | 2365 | CD2 | HIS A 298 | | 22.558 | | | | 7 |
| | 2366 | ND3 | HIS A 298 | | 21.779 | 48.538 | 52.205 | | 6 |
| MOTA | | CE1 | HIS A 298 | | 21.605 | | 52.522 | 1.00 31.84 | |
| MOTA | 2367 | CEL | HT2 W 730 | | 22.069 | | | 1.00 35.46 | 7 |
| ATOM | 2368 | NE2 | HIS A 298 | | | | | | 6 |
| ATOM | 2369 | С | HIS A 298 | | 25.213 | 46.697 | | | 8 |
| | | õ | HIS A 298 | | 25.471 | 46.405 | 54.133 | | |
| ATOM | 2370 | | | | 25.992 | | | 1.00 36.69 | 7 |
| ATOM | 2371 | N | PRO A.299 | | | | | | 6 |
| ATOM | 2372 | CD | PRO A 299 | | 25.680 | | | | 6 |
| | 2373 | CA | PRO A 299 | | 27.238 | 48.142 | | | 6 |
| ATOM | | | PRO A 299 | | 27.586 | 49.073 | 51.525 | | |
| MOTA | 2374 | CB | 200 M 233 | | 26.216 | 49.399 | 50.954 | 1.00 37.76 | 6 |
| ATOM | 2375 | CG | PRO A 299 | | | | | | 6 |
| MCTA | 2376 | С | PRO A 299 | | 27.045 | 48.886 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | |
| A+ | | | | | | | | | |

| ATOM 2319 N TYR A 3000 26.051 49.763 54.026 1.00 32.89 / ATOM 2319 CA TYR A 3000 24.496 51.377 55.009 1.00 35.56 6 6 ATOM 2381 CC TYR A 3000 24.496 51.377 55.009 1.00 35.596 6 ATOM 2381 CC TYR A 3000 25.370 52.367 52.842 1.00 39.76 6 ATOM 2381 CC TYR A 3000 25.370 52.367 52.842 1.00 39.76 6 ATOM 2383 CEI TYR A 3000 24.098 53.405 53.405 51.007 1.00 39.92 6 ATOM 2383 CEI TYR A 3000 24.098 54.615 33.405 51.007 1.00 39.92 6 ATOM 2386 CE TYR A 3000 24.098 54.615 33.405 51.007 1.00 39.92 6 ATOM 2386 CE TYR A 3000 24.098 54.612 52.161 1.00 38.09 6 ATOM 2386 CE TYR A 3000 24.987 55.634 51.251 1.00 37.68 8 ATOM 2388 C TYR A 3000 25.497 49.546 56.369 1.00 31.10 6 ATOM 2389 C TYR A 3000 25.497 49.546 56.369 1.00 31.10 6 ATOM 2389 C TYR A 3000 24.698 57.644 51.251 1.00 32.55 7 ATOM 2388 C TYR A 3001 24.661 48.541 56.125 1.00 32.55 7 ATOM 2389 C TYR A 3001 24.661 48.541 56.125 1.00 32.55 7 ATOM 2389 C TYR A 3001 24.661 48.541 56.125 1.00 32.55 7 ATOM 2391 CA ALA A 301 23.216 46.602 56.624 1.00 24.69 6 ATOM 2391 CA ALA A 301 23.216 46.502 56.524 1.00 24.69 6 ATOM 2393 C B ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2393 C B ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2393 C B ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 23.216 56.624 1.00 24.69 6 ATOM 2395 C B ALA A 301 24.69 ATOM 2395 C B ATOM 2395 C B ATOM 2 | ATOM | 2377 | | A 299 | 27.781 | 48.670 49.763 | 54.963 54.026 | 1.00 33.67 1.00 32.69 | 8 7 |
|---|------|------|---------|------------------|--------|------------------|------------------|--------------------------|--------|
| ATOM 2380 CB TYR A 3000 24, 496 51, 377 55, 009 1, 00 35, 56 6 ATOM 2381 CG TYR A 300 24, 648 52, 524 54, 028 1, 00 35, 56 6 ATOM 2383 CEI TYR A 300 25, 370 52, 367 52, 842 1, 00 39, 92 6 ATOM 2385 CEZ TYR A 300 24, 165 53, 405 51, 907 1, 00 39, 92 6 ATOM 2385 CEZ TYR A 300 24, 165 53, 405 51, 907 1, 00 36, 78 6 ATOM 2385 CEZ TYR A 300 24, 165 53, 405 51, 907 1, 00 36, 78 6 ATOM 2385 CEZ TYR A 300 24, 165 53, 405 51, 907 1, 00 36, 78 6 ATOM 2386 CZ TYR A 300 24, 165 53, 405 51, 100 1, 00 36, 78 6 ATOM 2386 CZ TYR A 300 24, 823 54, 612 52, 161 1, 00 37, 68 8 ATOM 2389 C TYR A 300 24, 823 54, 612 52, 161 1, 00 37, 68 8 ATOM 2389 C TYR A 300 25, 497 49, 546 56, 359 1, 00 37, 68 8 ATOM 2399 N A AA A 301 24, 323 47, 541 57, 145 1, 00 31, 64 6 ATOM 2391 CB ALA A 301 24, 323 47, 541 57, 145 1, 00 31, 64 6 ATOM 2392 CB ALA A 301 22, 164 6, 602 56, 624 1, 00 24, 69 6- ATOM 2393 C ALA A 301 25, 539 46, 727 75, 7552 1, 00 30, 06 6- ATOM 2393 C ALA A 301 25, 539 46, 727 75, 7552 1, 00 30, 06 6- ATOM 2395 N LEU A 302 26, 223 46, 192 56, 557 1, 00 30, 05 6 ATOM 2395 CB LEU A 302 27, 404 45, 303 56, 795 1, 00 30, 05 6 ATOM 2399 CD LEU A 302 28, 012 45, 002 55, 541 1, 00 31, 64 6 ATOM 2399 CD LEU A 302 28, 014 45, 303 56, 795 1, 00 30, 01 6 ATOM 2399 CD LEU A 302 28, 418 46, 136 57, 663 1, 00 31, 83 6 ATOM 2400 CD LEU A 302 29, 417 43, 781 53, 888 1, 00 32, 23 6 ATOM 2401 C LEU A 302 29, 417 43, 781 53, 888 1, 00 32, 23 6 ATOM 2402 C LEU A 302 28, 496 47, 297 557, 497 1, 00 31, 83 6 ATOM 2405 C B ALA A 301 30, 304 64, 577 75, 577, 577 1, 00 31, 63 6 ATOM 2406 C ALA A 303 30, 40 47, 541 57, 577, 577 1, 00 31, 63 6 ATOM 2407 C ALA A 303 30, 40 47, 541 57, 577 1, 57 | | | | | | | | 1.00 32.97 | |
| ATOM 2381 CG TYR A 300 24.648 52.524 54.02 3.00 38.37 6 6 7 7 7 7 7 7 1.00 38.97 6 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 7 1 | | | CB TYR | A 300 | 24.496 | | | 1.00 35.56 | |
| ATOM 2382 CDI TYR A 300 | | | CG TYR | A 300 | | | | | |
| ATOM 2384 CD2 TYR À 300 24.086 53.752 54.259 1.00 35.78 6 ATOM 2385 CEZ TYR À 300 24.098 54.793 53.334 1.00 36.78 6 ATOM 2386 CZ TYR À 300 24.098 54.793 53.334 1.00 37.68 8 ATOM 2387 OH TYR À 300 24.927 55.634 51.251 1.00 37.68 8 ATOM 2389 C TR À 300 24.927 55.634 51.251 1.00 37.68 8 ATOM 2389 O TYR À 300 25.497 49.546 56.359 1.00 37.68 8 ATOM 2399 N ALA À 301 24.661 48.541 56.125 1.00 32.55 7 ATOM 2391 CA ALA À 301 24.461 48.541 56.125 1.00 32.55 7 ATOM 2392 CB ALA À 301 24.46.602 56.624 1.00 31.64 6 ATOM 2393 C BLA À 301 25.539 46.727 57.552 1.00 31.64 6 ATOM 2393 C BLA À 301 25.539 46.727 57.552 1.00 31.64 6 ATOM 2395 N LEU À 302 26.223 46.192 56.557 1.00 31.91 8 ATOM 2395 C BLEU À 302 27.404 45.383 56.795 1.00 31.91 8 ATOM 2397 CB LEU À 302 28.012 45.002 55.441 1.00 31.83 6 ATOM 2399 CD1 LEU À 302 29.315 44.223 55.323 1.00 30.01 6 ATOM 2399 CD1 LEU À 302 29.315 45.507 57.652 1.00 30.05 6 ATOM 2399 CD1 LEU À 302 29.315 47.253 53.324 1.00 30.06 6 ATOM 2400 CD2 LEU À 302 29.315 47.253 53.324 1.00 30.01 6 ATOM 2401 C LEU À 302 29.315 47.254 1.00 30.05 6 ATOM 2402 O LEU À 302 29.315 47.254 1.00 30.05 6 ATOM 2403 N ALA À 301 30.288 482 47.299 57.179 1.00 22.99 6 ATOM 2404 CA ALA À 303 30.288 482 47.299 57.179 1.00 27.68 8 ATOM 2406 C ALA À 303 30.288 482 47.299 57.179 1.00 27.08 8 ATOM 2408 N ARG À 304 28.828 49.054 59.472 1.00 27.68 8 ATOM 2408 N ARG À 304 28.828 49.054 59.472 1.00 22.09 6 ATOM 2408 N ARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2410 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2410 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2420 C ALA À 303 30.486 49.052 69.91 1.00 22.09 6 ATOM 2421 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2421 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2421 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2421 C BARG À 304 28.838 49.054 59.472 1.00 22.09 6 ATOM 2421 C BARG À 304 28.838 49.054 59.472 1.00 22.00 6 ATOM 2422 C C ALA À 305 28.838 49.054 59.797 1.00 22.00 6 ATOM 2422 C C ALA À 306 30.448 49.506 50.558 59.992 1.00 22.07 6 A | | | | | | | | | |
| ATOM 2385 CEZ TYR A 300 | | | | | | | 54.259 | 1.00 35.92 | |
| ATOM 2386 CZ TYR A 300 24.823 \$4.612 \$21.611 1.00 37.88 8 ATOM 2387 OH TYR A 300 24.927 \$5.634 \$1.251 1.00 37.88 8 ATOM 2388 C TYR A 300 25.497 49.546 \$6.369 1.00 31.10 6 ATOM 2389 N ALA A 301 24.661 48.541 \$5.125 1.00 37.55 7 ATOM 2390 N ALA A 301 24.661 48.541 \$5.125 1.00 37.55 7 ATOM 2392 CB ALA A 301 24.661 48.541 \$5.125 1.00 37.55 7 ATOM 2393 C B ALA A 301 24.661 48.541 \$5.125 1.00 37.55 7 ATOM 2393 C B ALA A 301 24.621 48.541 \$5.125 1.00 31.64 6 ATOM 2393 C B ALA A 301 25.539 46.727 75.552 1.00 30.06 6 ATOM 2393 C B ALA A 301 25.539 46.727 75.552 1.00 30.06 6 ATOM 2395 C B ALE A 302 27.404 \$45.383 \$5.795 1.00 30.96 6 ATOM 2395 C B LEU A 302 27.404 \$45.383 \$5.795 1.00 30.55 6 ATOM 2396 C B LEU A 302 29.315 \$44.223 \$5.323 1.00 30.01 6 ATOM 2398 C B LEU A 302 29.315 \$44.223 \$5.323 1.00 30.01 6 ATOM 2399 CDI LEU A 302 29.315 \$44.223 \$5.323 1.00 30.01 6 ATOM 2399 CDI LEU A 302 29.491 \$43.781 \$5.888 1.00 32.09 6 ATOM 2400 CDZ LEU A 302 28.418 \$40.376 1.00 27.68 ATOM 2402 C LEU A 302 28.718 \$45.077 \$5.762 1.00 32.23 6 CATOM 2401 C LEU A 302 28.418 \$40.136 57.663 1.00 27.68 ATOM 2402 C LEU A 302 28.418 \$40.136 57.663 1.00 27.68 ATOM 2402 C LEU A 302 28.796 \$45.675 \$8.746 1.00 27.68 ATOM 2405 CB ALA A 303 29.818 \$48.119 \$7.877 1.00 25.00 6 ATOM 2407 C ALA A 303 29.818 \$48.119 \$7.877 1.00 25.00 6 ATOM 2407 C ALA A 303 29.818 \$48.119 \$7.877 1.00 25.00 6 ATOM 2407 C ALA A 303 30.026 \$49.424 \$7.137 1.00 23.62 6 ATOM 2407 C ALA A 303 30.026 \$49.424 \$7.137 1.00 23.62 6 ATOM 2407 C ALA A 303 30.088 \$48.015 \$5.9472 1.00 24.06 7 ATOM 2401 C ALA A 303 30.886 \$49.054 \$5.9472 1.00 24.06 7 ATOM 2402 C ALA A 303 30.886 \$49.054 \$5.9472 1.00 24.06 7 ATOM 2401 C B ARG A 304 22.893 \$1.253 \$60.801 1.00 24.379 6 ATOM 2401 C B ARG A 304 22.893 \$1.253 \$60.801 1.00 24.379 6 ATOM 2402 C ALA A 303 304 26.202 \$60.758 1.00 23.996 6 ATOM 2402 C ALA A 303 304 26.203 \$60.801 1.00 24.33 6 ATOM 2411 C B ARG A 304 22.894 \$9.054 \$4.961 1.00 24.96 6 ATOM 2412 C B ALA A 303 304 26.203 \$9.505 \$1.257 \$1.00 24.00 \$7.00 \$1.00 \$1.00 \$1.00 \$1.00 \$1.00 \$1. | | | | | | 54.793 | | 1.00 36.78 | |
| ATOM 2388 C TYR À 300 | | | CZ .TYR | A 300 | | | | 1.00 38.09 | |
| ATOM 2388 C TYR A 300 | | 2387 | | A 300 | 24.927 | | | | 6 |
| ATOM 2390 N ALA A 301 24.361 56.125 1.00 32.95 6 ATOM 2391 CA ALA A 301 24.323 47.541 57.145 1.00 31.64 6 ATOM 2392 CB ALA A 301 23.216 46.502 56.624 1.00 24.69 6 ATOM 2393 C ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2394 O ALA A 301 25.848 46.579 58.734 1.00 31.91 8 ATOM 2395 N LEU A 302 27.404 45.383 56.795 1.00 28.94 7 ATOM 2396 CA LEU A 302 27.404 45.383 56.795 1.00 30.55 6 ATOM 2397 CB LEU A 302 29.491 43.083 56.795 1.00 30.01 6 ATOM 2398 CG LEU A 302 29.491 43.781 53.888 1.00 32.09 6 ATOM 2399 CD1 LEU A 302 29.491 43.781 53.888 1.00 32.09 6 ATOM 2400 CD2 LEU A 302 29.491 43.781 53.888 1.00 32.09 6 ATOM 2401 C LEU A 302 28.418 46.136 57.663 1.00 29.79 6 ATOM 2402 O LEU A 302 28.916 56.76 58.746 1.00 27.68 8 ATOM 2402 O LEU A 302 28.842 47.299 57.179 1.00 27.68 8 ATOM 2403 N ALA A 303 28.842 47.299 57.179 1.00 27.68 8 ATOM 2404 CA ALA A 303 29.397 48.397 59.305 1.00 25.00 6 ATOM 2405 CB ALA A 303 30.026 49.424 57.137 1.00 23.62 6 ATOM 2406 C ALA A 303 30.026 49.424 57.137 1.00 23.62 6 ATOM 2407 O ALA A 303 30.088 48.015 50.248 1.00 24.06 7 ATOM 2408 N ARG A 304 27.994 49.382 60.810 1.00 24.37 6 ATOM 2409 CA ARG A 304 27.994 49.382 60.810 1.00 24.37 6 ATOM 2401 CB ARG A 304 27.994 49.382 60.781 1.00 23.62 60 ATOM 2401 CB ARG A 304 27.994 49.382 60.810 1.00 24.37 6 ATOM 2402 CB ARG A 304 27.994 49.382 60.810 1.00 24.37 6 ATOM 2401 CB ARG A 304 27.974 49.382 60.810 1.00 24.37 6 ATOM 2411 CC ARG A 304 27.777 48.142 61.691 1.00 24.37 6 ATOM 2412 CD ARG A 304 27.777 48.142 61.691 1.00 24.37 6 ATOM 2412 CB ARG A 304 27.777 48.142 61.691 1.00 24.37 6 ATOM 2413 N R ARG A 304 27.777 48.192 60.810 1.00 22.34 8 ATOM 2410 CB ARG A 304 27.777 48.192 60.810 1.00 22.34 8 ATOM 2411 CC ARG A 304 22.893 51.573 61.110 1.00 34.36 6 ATOM 2412 CD ARG A 304 22.893 51.573 61.110 1.00 24.37 6 ATOM 2412 CD ARG A 304 22.893 51.573 61.110 1.00 24.30 6 ATOM 2412 CD ARG A 304 22.893 51.573 61.110 1.00 24.36 6 ATOM 2421 CD ARG A 304 22.893 51.573 61.110 1.00 24.20 6 ATOM 2422 CD ALA A 305 26.994 47.132 61.20 1.00 22.34 8 ATOM 2423 | | | | | 26.062 | | 57.440 | 1.00 30.62 | |
| ATOM 2391 CA ALA A 301 23.216 46.602 55.624 1.00 24.69 6. ATOM 2392 CB ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2393 C ALA A 301 25.539 46.727 57.552 1.00 30.06 6 ATOM 2395 N LEU A 302 27.404 45.383 56.797 5.8734 1.00 31.91 8 ATOM 2395 N LEU A 302 27.404 45.383 56.797 5.00 30.055 6 ATOM 2396 CA LEU A 302 28.012 45.002 55.441 1.00 31.83 6 ATOM 2397 CB LEU A 302 29.315 44.223 55.332 1.00 30.01 6 ATOM 2399 CD LEU A 302 29.315 44.223 55.323 1.00 30.01 6 ATOM 2399 CD LEU A 302 29.315 46.075 5.762 1.00 32.09 6 ATOM 2400 CD2 LEU A 302 29.315 46.075 5.762 1.00 32.09 6 ATOM 2400 CD2 LEU A 302 29.315 46.075 5.762 1.00 32.09 6 ATOM 2400 CD2 LEU A 302 29.315 46.075 5.762 1.00 32.23 6 ATOM 2402 O LEU A 302 28.796 45.676 58.746 1.00 27.68 8 ATOM 2402 O LEU A 302 28.796 45.676 58.746 1.00 27.68 8 ATOM 2402 O LEU A 303 30.88 82 47.299 57.179 1.00 27.92 7 ATOM 2401 CA ALA A 303 29.818 48.119 57.877 1.00 25.00 6 ATOM 2402 O LEU A 303 29.818 48.119 57.877 1.00 25.00 6 ATOM 2404 CA ALA A 303 30.088 48.015 60.248 1.00 22.09 6 ATOM 2405 CB ALA A 303 30.088 48.015 60.248 1.00 25.06 6 ATOM 2405 CB ALA A 303 30.088 48.015 60.248 1.00 22.09 6 ATOM 2405 CB ALA A 303 30.088 48.015 60.248 1.00 22.09 6 ATOM 2401 CB ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2401 CB ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2401 CB ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2410 CB ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2411 CG ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2412 CD ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2412 CD ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2412 CD ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2412 CD ARG A 304 28.333 48.099 60.156 1.00 29.96 6 ATOM 2412 CD ARG A 304 22.893 51.253 60.359 60.156 1.00 29.96 6 ATOM 2412 CB ARG A 304 22.893 51.253 60.359 60.156 1.00 22.379 6 ATOM 2412 CB ARG A 304 22.893 51.253 60.369 60.248 1.00 26.208 7 ATOM 2412 CB ALA A 305 26.804 47.295 60.810 1.00 24.24 6 ATOM 2418 NHL ARG A 304 22.893 51.253 60.359 60.22 1.00 22.344 6 ATOM 2420 CB ALA | | | N ALA | A 301 | 24.661 | | | 1.00 32.55 | |
| ATOM 2393 C ALA A 301 | | 2391 | | A 301 | 24.323 | | | | |
| ATOM 2394 | | | | | 25.539 | | 57.552 | 1.00 30.06 | |
| ATOM 2395 N LEU A 302 26.223 46.192 56.397 1.00 20.55 6 ATOM 2396 CA LEU A 302 28.012 45.002 55.441 1.00 31.83 6 ATOM 2397 CB LEU A 302 29.315 44.223 55.323 1.00 30.01 6 ATOM 2399 CDI LEU A 302 29.491 43.781 53.888 1.00 32.09 6 ATOM 2400 CD2 LEU A 302 28.796 45.676 55.7663 1.00 22.23 6 ATOM 2401 C LEU A 302 28.796 45.676 58.746 1.00 27.68 8 ATOM 2402 O LEU A 302 28.796 45.676 58.746 1.00 27.92 7 ATOM 2403 N ALA A 303 28.842 47.299 57.179 1.00 27.92 7 ATOM 2404 CA ALA A 303 29.818 48.119 57.877 1.00 25.06 6 ATOM 2405 CB ALA A 303 30.026 49.424 57.137 1.00 23.62 6 ATOM 2406 C ALA A 303 30.088 48.015 60.248 1.00 23.99 6 ATOM 2407 O ALA A 303 30.088 48.015 60.248 1.00 23.99 6 ATOM 2409 CA ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2409 CA ARG A 304 27.794 49.382 60.810 1.00 24.37 6 ATOM 2410 CB ARG A 304 26.328 51.257 59.815 1.00 23.99 6 ATOM 2411 CG ARG A 304 26.328 51.257 59.815 1.00 23.99 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2411 CA ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2416 NAZ ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2417 C ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2418 O ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2419 N ALA A 305 26.994 47.132 61.221 1.00 24.23 48 ATOM 2421 CD ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 O ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2417 C ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 O ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2421 CD ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2421 CD ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2422 CD ALA 305 26.994 47.132 61.221 1.00 24.24 6 ATOM 2423 O ALA A 305 26.994 47.132 61.221 1.00 24.24 6 ATOM 2424 CD TAPA 306 30.464 42.503 59.995 1.00 24.36 6 ATOM 2425 CD TAPA 306 30.464 42.503 59.995 1.00 24.35 6 ATOM 2 | | | O ALA | A 301 | 25.848 | | | | |
| ATOM 2396 CA LEU A 302 28.012 43.022 55.441 1.00 31.83 6 ATOM 2398 CG LEU A 302 29.315 44.223 55.323 1.00 30.01 6 ATOM 2399 CD1 LEU A 302 30.475 45.077 55.762 1.00 32.23 6 ATOM 2400 CD2 LEU A 302 28.418 46.136 57.663 1.00 29.79 6 ATOM 2401 C LEU A 302 28.418 46.136 57.663 1.00 29.79 6 ATOM 2402 O LEU A 302 28.796 45.676 58.746 1.00 27.58 8 ATOM 2403 N ALA A 303 28.842 47.299 57.179 1.00 27.92 7 ATOM 2404 C A ALA A 303 29.818 48.119 57.877 1.00 25.00 6 ATOM 2405 CB ALA A 303 30.026 49.424 57.137 1.00 25.00 6 ATOM 2406 C ALA A 303 30.026 49.424 57.137 1.00 25.00 6 ATOM 2407 O ALA A 303 30.088 48.015 60.248 1.00 24.06 7 ATOM 2408 N ARG A 304 28.258 49.054 59.472 1.00 24.06 7 ATOM 2409 CA ARG A 304 26.420 50.052 60.758 1.00 28.797 6 ATOM 2411 CG ARG A 304 26.420 50.052 60.758 1.00 28.797 6 ATOM 2412 CD ARG A 304 25.106 52.089 60.156 1.00 28.77 6 ATOM 2413 NE ARG A 304 25.106 52.089 60.156 1.00 28.77 6 ATOM 2414 CZ ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2417 C ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2416 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2417 C ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2416 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2417 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2418 NAIL ARG A 304 22.893 51.573 61.110 1.00 36.37 7 ATOM 2420 CA ALA A 305 26.894 47.132 61.221 1.00 24.36 6 ATOM 2421 C BARG A 304 27.727 48.142 61.691 1.00 24.36 6 ATOM 2422 C BALA 305 26.891 47.132 61.221 1.00 24.36 6 ATOM 2423 O ALA 3.305 26.891 47.132 61.221 1.00 24.36 6 ATOM 2424 N TRP 3.306 30.484 44.961 61.411 1.00 22.79 6 ATOM 2425 C BTRP A 306 30.484 44.961 61.411 1.00 22.79 6 ATOM 2426 C BTRP A 306 30.486 42.503 59.992 1.00 26.38 6 ATOM 2427 CG TRP A 306 30.444 44.72 66.1691 1.00 24.20 6 ATOM 2428 CD TRP A 306 30.446 44.270 61.764 1.00 24.20 6 ATOM 2433 CZ TRP A 306 31.484 48.796 63.100 | | | N LEU | A 302 | | | | | |
| ATOM 2398 CG LEU A 302 | MOTA | | | | | | | 1.00 31.83 | 6 |
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| ATOM 2411 CD ARG A 304 | | | CB ARG | ; A 304 · | | | 59.815 | 1.00 28.77 | |
| ATOM 2413 NE ARG A 304 22.893 51.233 60.359 1.00 38.43 6 ATOM 2415 NH1 ARG A 304 22.893 51.573 61.110 1.00 37.01 6 ATOM 2416 NH2 ARG A 304 21.896 50.719 61.269 1.00 34.36 7 ATOM 2417 C ARG A 304 27.727 48.142 61.691 1.00 24.24 6 ATOM 2419 N ALA A 305 26.994 47.132 61.221 1.00 24.51 7 ATOM 2421 CB ALA A 305 26.801 45.883 61.959 1.00 22.70 6 ATOM 2422 C ALA A 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2422 C ALA A 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2423 O ALA A 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2424 N TRP A 306 30.244 44.270 61.764 1.00 24.33 6 ATOM 2425 CA TRP A 306 30.244 44.270 61.764 1.00 24.33 6 ATOM 2427 CG TRP A 306 30.604 42.503 59.952 1.00 27.96 6 ATOM 2429 CE2 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2429 CE2 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2429 CE2 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2429 CE2 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2430 CE3 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2430 CE3 TRP A 306 30.861 42.013 58.629 1.00 26.93 6 ATOM 2431 CD1 TRP A 306 30.450 39.904 57.441 1.00 24.51 6 ATOM 2432 NEI TRP A 306 31.462 42.563 57.490 1.00 23.00 6 ATOM 2433 CE2 TRP A 306 31.462 42.563 57.490 1.00 23.00 6 ATOM 2433 CE2 TRP A 306 31.462 42.563 57.490 1.00 25.62 7 ATOM 2434 CC3 TRP A 306 31.462 42.563 57.490 1.00 25.37 6 ATOM 2433 CE2 TRP A 306 31.462 42.563 57.490 1.00 25.37 6 ATOM 2433 CE2 TRP A 306 31.462 42.563 57.490 1.00 25.37 6 ATOM 2433 CC2 TRP A 306 31.462 40.465 56.315 1.00 24.51 6 ATOM 2433 CC2 TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2435 CC2 TRP A 306 31.548 41.784 56.343 1.00 25.07 8 ATOM 2435 CC2 TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2436 C TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2437 C TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 24410 CB TRP A 307 31.994 49.119 61 | | | | A 304 | 25.106 | | | 1.00 29.96 | |
| ATOM 2415 NH1 ARG A 304 22.854 52.757 61.713 1.00 36.37 7 ATOM 2415 NH1 ARG A 304 21.896 50.719 61.269 1.00 34.36 7 ATOM 2417 C ARG A 304 27.727 48.142 61.691 1.00 24.24 6 ATOM 2419 N ALA A 305 26.894 47.132 61.221 1.00 24.51 7 ATOM 2419 N ALA A 305 26.801 45.883 61.959 1.00 22.70 6 ATOM 2421 CB ALA A 305 25.880 44.960 61.175 1.00 18.13 6 ATOM 2422 C ALA 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2422 C ALA 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2423 O ALA 305 28.237 44.725 63.506 1.00 21.51 8 ATOM 2424 N TRP 306 29.016 44.961 61.411 1.00 22.79 7 ATOM 2424 N TRP A 306 30.244 44.270 61.764 1.00 24.33 6 ATOM 2425 CA TRP A 306 30.244 44.270 ATOM 2427 CG TRP A 306 30.604 42.503 59.952 1.00 27.96 6 ATOM 2428 CD2 TRP A 306 30.861 42.013 58.629 1.00 24.93 6 ATOM 2429 CE2 TRP A 306 30.366 40.688 ATOM 2429 CE2 TRP A 306 30.366 40.688 55.8570 1.00 24.96 6 ATOM 2431 CD1 TRP A 306 30.366 40.688 57.490 1.00 24.96 6 ATOM 2431 CD1 TRP A 306 30.440 42.503 59.952 1.00 27.96 6 ATOM 2431 CD1 TRP A 306 30.464 42.503 59.952 1.00 27.96 6 ATOM 2431 CD1 TRP A 306 30.366 40.688 57.490 1.00 24.96 6 ATOM 2431 CD1 TRP A 306 30.366 40.688 57.490 1.00 24.96 6 ATOM 2432 NEI TRP A 306 30.450 39.9904 57.414 1.00 24.51 6 ATOM 2433 CC2 TRP A 306 31.462 42.563 57.490 1.00 25.37 6 ATOM 2434 CC3 TRP A 306 31.462 40.465 56.315 1.00 25.37 6 ATOM 2435 CH2 TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2435 CH2 TRP A 306 31.903 46.427 62.575 1.00 25.07 8 ATOM 2438 N THR A 307 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.908 44.570 63.464 1.00 27.91 6 ATOM 2441 CB1 THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 CB1 THR A 307 31.99 | | 2413 | NE ARG | A 304 | | | | 1.00 37.01 | |
| ATOM 2416 NH2 ARG A 304 | | | CZ ARC | A 304 | | | | 1.00 36.37 | |
| ATOM 2417 C ARG A 304 27.727 48.142 61.691 1.00 22.34 8 ATOM 2418 O ARG A 304 28.343 48.099 62.762 1.00 22.34 8 ATOM 2419 N ALA A 305 26.994 47.132 61.221 1.00 24.51 7 ATOM 2420 CA ALA A 305 26.891 45.883 61.959 1.00 22.70 6 ATOM 2421 CB ALA A 305 25.880 44.960 61.175 1.00 18.13 6 ATOM 2422 C ALA 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2423 O ALA 305 28.089 45.142 62.351 1.00 23.33 6 ATOM 2424 N TRP 306 29.016 44.961 61.411 1.00 22.79 7 ATOM 2425 CA TRP A 306 30.244 44.270 61.764 1.00 24.33 6 ATOM 2426 CB TRP A 306 31.029 43.842 60.524 1.00 26.93 6 ATOM 2427 CG TRP A 306 30.861 42.013 58.629 1.00 27.96 6 ATOM 2428 CD2 TRP A 306 30.861 42.013 58.629 1.00 26.38 6 ATOM 2429 CE2 TRP A 306 30.366 40.688 58.570 1.00 24.96 6 ATOM 2431 CD1 TRP A 306 31.462 42.563 57.490 1.00 23.00 6 ATOM 2432 NE1 TRP A 306 31.462 42.563 57.490 1.00 23.00 6 ATOM 2433 CZ2 TRP A 306 30.450 39.904 57.414 1.00 24.51 6 ATOM 2434 CZ3 TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2435 CH2 TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2436 C TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2437 C TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2438 N THR A 307 31.994 49.119 61.799 1.00 20.7.91 6 ATOM 2439 CA THR A 307 31.998 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.998 44.570 63.464 1.00 27.91 6 ATOM 2439 CA THR A 307 31.998 44.570 63.461 1.00 27.96 6 ATOM 2439 CA THR A 307 31.998 44.570 63.461 1.00 27.96 6 ATOM 2439 CA THR A 307 31.998 44.570 63.160 1.00 27.96 6 ATOM 2439 CA THR A 307 31.998 44.570 63.160 1.00 27.96 6 ATOM 2439 CA THR A 307 31.998 44.570 63.160 1.00 27.96 6 ATOM 2440 CB THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 CG THR A 307 31.994 49.119 61.799 1.00 30.17 8 | | _ | NH1 ARC | A 304 | | 50.719 | | 1.00 34.36 | |
| ATOM 2419 N ALA A 305 | | | C ARC | 3 A 304 | | | | | |
| ATOM 2429 CA ALA A 305 | | | | 3 A 304 | | | | 1.00 24.51 | 7 |
| ATOM 2421 CB ALA A 305 | | | | | | | | | |
| ATOM 2422 C ALA 305 28.089 45.142 62.331 1.00 22.79 7 ATOM 2423 O ALA 305 29.016 44.961 61.411 1.00 22.79 7 ATOM 2424 N TRP 306 30.244 44.270 61.764 1.00 24.33 6 ATOM 2425 CA TRP A 306 31.029 43.842 60.524 1.00 26.93 6 ATOM 2427 CG TRP A 306 30.604 42.503 59.952 1.00 27.96 6 ATOM 2428 CD2 TRP A 306 30.861 42.013 58.629 1.00 26.38 6 ATOM 2428 CD2 TRP A 306 30.366 40.688 58.570 1.00 24.96 ATOM 2429 CE2 TRP A 306 30.366 40.688 58.570 1.00 24.96 6 ATOM 2430 CE3 TRP A 306 31.462 42.563 57.490 1.00 23.00 6 ATOM 2431 CD1 TRP A 306 29.983 41.484 60.620 1.00 28.53 6 ATOM 2432 NE1 TRP A 306 29.887 40.392 59.797 1.00 25.62 7 ATOM 2433 CZ2 TRP A 306 30.450 39.904 57.414 1.00 24.51 6 ATOM 2434 CZ3 TRP A 306 31.548 41.784 56.343 1.00 25.37 6 ATOM 2436 CH2 TRP A 306 31.042 40.465 56.315 1.00 24.20 6 ATOM 2436 C TRP A 306 31.042 40.465 56.315 1.00 24.20 6 ATOM 2438 N THR A 307 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRP A 306 31.908 44.570 63.464 1.00 25.07 8 ATOM 2439 CA TRR A 307 31.785 47.323 63.415 1.00 27.91 6 ATOM 2439 CA TRR A 307 31.484 48.796 63.100 1.00 27.86 6 ATOM 2441 CB THR A 307 31.484 48.796 63.100 1.00 27.86 6 ATOM 2441 CG1 THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 CG1 THR A 307 31.994 49.704 64.137 1.00 24.72 6 | | | CB AL | A A 305 | | | | | |
| ATOM 2424 N TRP 306 ATOM 2424 N TRP A 306 ATOM 2425 CA TRP A 306 ATOM 2426 CB TRP A 306 ATOM 2427 CG TRP A 306 ATOM 2427 CG TRP A 306 ATOM 2428 CD2 TRP A 306 ATOM 2429 CE2 TRP A 306 ATOM 2429 CE2 TRP A 306 ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 CD2 TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2430 CB THR A 307 ATOM 2431 CB THR A 307 ATOM 2432 CB THR A 307 ATOM 2433 CB THR A 307 ATOM 2434 CB THR A 307 ATOM 2436 CB THR A 307 ATOM 2437 CB THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2430 CB THR A 307 ATOM 2431 CB THR A 307 ATOM 2432 CB THR A 307 ATOM 2433 CB THR A 307 ATOM 2434 CB THR A 307 ATOM 2437 CB THR A 307 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2430 CB THR A 307 ATOM 2431 CB THR A 307 ATOM 2441 CG1 THR A 307 | | | C AL | A 305 | | _ | | | |
| ATOM 2425 CA TRP A 306 ATOM 2426 CB TRP A 306 ATOM 2427 CG TRP A 306 ATOM 2428 CD2 TRP A 306 ATOM 2428 CD2 TRP A 306 ATOM 2429 CE2 TRP A 306 ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 CZ2 TRP A 306 ATOM 2437 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2437 CZ2 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2439 CA THR A 307 ATOM 2430 CA THR A 307 ATOM 2431 CCB THR A 307 ATOM 2441 CCB THR A | | | O AL | A . 305 B 306 | | | 61.411 | 1.00 22.79 | |
| ATOM 2426 CB TRP A 306 ATOM 2427 CG TRP A 306 ATOM 2428 CD2 TRP A 306 ATOM 2429 CE2 TRP A 306 ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 CD1 TRP A 306 ATOM 2438 CZ2 TRP A 306 ATOM 2439 CZ2 TRP A 306 ATOM 2430 CZ3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 CD1 TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2430 CB THR A 307 ATOM 2441 CG1 THR A | | - | | P A 306 | 30.244 | 44.270 | | 1.00 24.33 | |
| ATOM 2427 CG TRP A 306 ATOM 2428 CD2 TRP A 306 ATOM 2429 CE2 TRP A 306 ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 CD2 TRP A 306 ATOM 2438 CC2 TRP A 306 ATOM 2438 CC3 TRP A 306 ATOM 2439 CA TRP A 306 ATOM 2439 CA TRP A 307 ATOM 2430 CB TRP A 307 ATOM 2431 CD2 TRP A 307 ATOM 2432 CA TRP A 307 ATOM 2433 CA TRP A 307 ATOM 2434 CC3 TRP A 307 ATOM 2438 CA TRP A 307 ATOM 2439 CA TRP A 307 ATOM 2439 CA TRP A 307 ATOM 2439 CA TRP A 307 ATOM 2440 CB TRP A 307 ATOM 2441 CG1 TRP A 307 | | | CB TR | P A 306 | | | 60.524 | | |
| ATOM 2429 CE2 TRP A 306 ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 CG1 THR | | | | | | | | 1.00 26.38 | 6 |
| ATOM 2430 CE3 TRP A 306 ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 CG1 THR A 307 ATO | | | | | | 40.688 | 58.570 | 1.00 24.96 | |
| ATOM 2431 CD1 TRP A 306 ATOM 2432 NE1 TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 CG1 THR A 307 | | | CE3 TR | P A 306 | 31.462 | 42.563 | | | 6 |
| ATOM 2432 NEI TRP A 306 ATOM 2433 CZ2 TRP A 306 ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 OGI THR A 307 | | | CD1 TR | | | | | | 7 |
| ATOM 2434 CZ3 TRP A 306 ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2438 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 CG1 THR | MOTA | | | | | | | 1.00 24.51 | 6 |
| ATOM 2435 CH2 TRP A 306 ATOM 2436 C TRP A 306 ATOM 2437 O TRP A 306 ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 ATOM 2440 CB THR A 307 ATOM 2441 CG1 THR A 307 | | | | | | | 56.343 | 1.00 25.37 | 6 |
| ATOM 2436 C TRP A 306 31.129 49.100 63.464 1.00 25.07 8 ATOM 2438 N THR A 307 31.003 46.427 62.575 1.00 28.08 7 ATOM 2439 CA THR A 307 31.785 47.323 63.415 1.00 27.91 6 ATOM 2440 CB THR A 307 31.484 48.796 63.100 1.00 27.86 6 ATOM 2441 CG1 THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 CG1 THR A 307 32.120 49.704 64.137 1.00 24.72 6 | | | CH2 TR | P A 306 | | | | | 6 |
| ATOM 2437 O TRP A 306 31.508 44.327 62.575 1.00 28.08 7 ATOM 2438 N THR A 307 31.003 46.427 62.575 1.00 27.91 6 ATOM 2439 CA THR A 307 31.785 47.323 63.415 1.00 27.91 6 ATOM 2440 CB THR A 307 31.484 48.796 63.100 1.00 27.86 6 ATOM 2441 OG1 THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 OG1 THR A 307 32.120 49.704 64.137 1.00 24.72 6 | | 2436 | C TR | P A 306 | | | | 1.00 25.07 | 8 |
| ATOM 2438 N THR A 307 ATOM 2439 CA THR A 307 31.785 47.323 63.415 1.00 27.91 6 ATOM 2440 CB THR A 307 31.484 48.796 63.100 1.00 27.86 6 ATOM 2441 OGI THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 OGI THR A 307 32.120 49.704 64.137 1.00 24.72 6 | ATCM | | O TR | P A 306 | | · · · · | | 1.00 28.08 | 7 |
| ATOM 2440 CB THR A 307 31.484 48.796 63.100 1.00 30.17 8 ATOM 2441 OGI THR A 307 31.994 49.119 61.799 1.00 30.17 8 ATOM 2441 OGI THR A 307 32.120 49.704 64.137 1.00 24.72 6 | | | CA TH | R A 307 | 31.78 | 5 47.323 | 63.415 | | 6 |
| ATOM 2441 OG1 THR A 307 31.994 49.119 61.735 1.00 24.72 6 | | | CB TH | R A 307 | | | | - 44 34 47 | |
| | ATOM | 2441 | OG1 TH | R A 307 | | | | | |
| | ATOM | 2442 | CG2 TH | K A 30/ | | | • | | |

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| ATON 2444 C THR A 307 31. 441 47.041 64.863 1.00 29.35 6 ATON 2444 N LEW A 308 30.159 46.895 65.725 1.00 32.56 8 ATON 2446 CA LEU A 308 29.740 46.555 66.490 1.00 33.69 6 ATON 2447 CB LEU A 308 29.740 46.555 66.595 1.00 34.48 6 ATON 2448 CG LEU A 308 29.756 46.215 66.525 1.00 34.48 6 ATON 2448 CG LEU A 308 27.338 47.337 66.608 1.00 31.98 6 ATON 2448 CG LEU A 308 27.599 46.887 66.153 1.00 31.98 6 ATON 2448 CG LEU A 308 27.599 46.887 66.153 1.00 31.98 6 ATON 2445 CD LEU A 308 27.599 46.887 66.153 1.00 31.98 6 ATON 2451 C LEU A 308 27.599 46.887 66.153 1.00 31.98 6 ATON 2451 C LEU A 308 27.599 46.887 66.153 1.00 31.98 6 ATON 2451 C LEU A 308 31.230 44.262 66.208 1.00 35.78 7 ATON 2453 N LEA 309 31.230 44.262 66.208 1.00 35.78 7 ATON 2455 CB LEU A 308 31.230 44.262 66.208 1.00 35.78 7 ATON 2455 CB LEU A 308 31.230 44.262 66.208 1.00 35.78 7 ATON 2457 CG LILE A 309 31.733 40.695 65.799 1.00 31.21 6 ATON 2458 CG LILE A 309 31.733 40.695 65.799 1.00 31.21 6 ATON 2458 CG LILE A 309 32.589 43.238 66.772 1.00 34.25 6 ATON 2458 CG LILE A 309 32.589 43.238 66.772 1.00 34.25 6 ATON 2459 C LILE A 309 33.183 42.617 67.657 1.00 35.81 6 ATON 2460 C TRP A 310 33.183 42.617 67.657 1.00 35.81 6 ATON 2460 C TRP A 310 33.183 42.617 67.657 1.00 35.81 6 ATON 2460 C TRP A 310 33.183 42.617 67.657 1.00 35.26 6 ATON 2460 C TRP A 310 33.183 42.617 67.657 1.00 35.26 6 ATON 2461 N TRP A 310 33.183 42.617 67.657 1.00 35.26 6 ATON 2465 CG TRP A 310 35.150 45.311 65.075 1.00 32.51 6 ATON 2465 CG TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATON 2465 CG TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATON 2465 CG TRP A 310 37.076 44.620 65.274 1.00 32.91 6 ATON 2467 CG TRP A 310 37.076 44.620 65.274 1.00 32.91 6 ATON 2467 CG TRP A 310 37.679 44.620 65.274 1.00 32.92 93 6 ATON 2470 C TRP A 310 37.679 44.620 65.274 1.00 32.92 93 6 ATON 2470 C TRP A 310 37.679 44.620 65.274 1.00 32.92 93 6 ATON 2467 C C TRP A 310 37.679 44.620 65.274 1.00 32.92 93 6 ATON 2467 C C TRP A 310 37.076 44.620 65.274 1.00 37.576 65.00 65.00 65.00 65.00 65.00 65.00 65.00 65.00 | | | | | | | | | | | | \0.3E | c |
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| AFTON 2444 O | ATOM | 2443 | С | THR A | 307 | | | | | | | | |
| ATOM 2445 N LEU A 308 30.199 46.555 66.490 1.00 33.69 6 | | _ | | THR A | .307 | | | | | | | | |
| ATOM 2446 CA LEU A 308 29, 740 40.333 66.252 1.00 34.78 6 6 6 6 6 6 6 6 6 | | | N | LEU A | 308 | | | | | | | | |
| ATOM 2447 CB LEU A 308 ATOM 2448 CG LEU A 308 ATOM 2449 CD LEU A 308 ATOM 2449 CD LEU A 308 ATOM 2449 CD LEU A 308 ATOM 2450 CD2 LEU A 308 ATOM 2451 C LEU A 308 ATOM 2451 C LEU A 308 ATOM 2451 C LEU A 308 ATOM 2452 O LEU A 308 ATOM 2452 O LEU A 308 ATOM 2453 N ILE A 309 ATOM 2453 N ILE A 309 ATOM 2455 CB LLE A 309 ATOM 2455 CB LLE A 309 ATOM 2455 CB LLE A 309 ATOM 2455 CC2 LLE A 308 ATOM 2456 CC2 LLE A 308 ATOM 2457 CG1 LLE A 309 ATOM 2457 CG1 LLE A 309 ATOM 2458 CD1 LLE A 309 ATOM 2458 CD1 LLE A 309 ATOM 2459 C LLE A 309 ATOM 2450 CD1 LTE A 309 ATOM 2451 CD1 ATOM 2450 CD2 | | | CA | LEU A | 308 | - | | | | 66.490 | | | |
| ATOM 2448 CG LEU A 308 27,388 47,337 68.153 1.00 31.98 6 | | | CB | LEU A | 308 | | | | | | | | |
| ATOM 2449 CPI LEU A 308 | | | CG | LEU A | 308 | | | | | | | | |
| ATOM 2450 CD2 LEU A 308 | | 2449 | CD1 | LEU A | 308 | | | - | | 66 924 | | | |
| ATOM 2451 C LEU À 308 31.230 45.417 67.975 1.00 33.75 8 ATOM 2452 O LEU À 308 30.423 44.262 66.208 1.00 35.87 6 ATOM 2454 CÀ LE À 309 30.423 44.262 66.208 1.00 35.87 6 ATOM 2455 CB LE À 309 31.108 43.017 66.540 1.00 35.87 6 ATOM 2455 CG LE À 309 31.733 40.695 65.799 1.00 31.21 6 ATOM 2456 CG2 LLE À 309 31.733 40.695 65.799 1.00 31.21 6 ATOM 2457 CG1 LLE À 309 28.726 41.014 66.407. 1.00 25.04 6 ATOM 2459 C LLE À 309 32.589 43.238 66.772 1.00 35.81 6 ATOM 2450 C LLE À 309 33.183 42.617 67.657 1.00 38.19 8 ATOM 2450 C LLE À 309 33.183 42.617 67.657 1.00 38.19 8 ATOM 2451 N TRP À 310 33.197 44.111 65.977 1.00 36.10 7 ATOM 2461 N TRP À 310 35.150 45.311 65.075 1.00 32.26 6 ATOM 2462 CÀ TRP À 310 35.150 45.311 65.075 1.00 32.26 6 ATOM 2464 CG TRP À 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CEZ TRP À 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CEZ TRP À 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2468 CD1 TRP À 310 37.7206 46.65 86.520 1.00 30.79 6 ATOM 2468 CD1 TRP À 310 37.7206 46.65 96.536 1.00 29.37 7 ATOM 2468 CD1 TRP À 310 37.7206 46.65 96.536 1.00 29.37 7 ATOM 2470 CZZ TRP À 310 38.892 45.330 65.474 1.00 28.42 6 ATOM 2471 CZ3 TRP À 310 38.892 45.330 65.474 1.00 28.06 6 ATOM 2471 CZ3 TRP À 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2472 CH2 TRP À 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2473 C TRP À 310 31.349 49.401 67.796 1.00 32.82 6 ATOM 2474 O TRP À 310 31.349 49.401 67.796 1.00 32.82 6 ATOM 2475 N CYS À 311 33.139 44.91 47.97 1.00 33.86 6 ATOM 2476 CA CYS À 311 33.439 49.401 67.796 1.00 32.82 6 ATOM 2477 CB CYS À 311 33.439 49.401 67.796 1.00 32.82 6 ATOM 2489 C C CYS À 311 33.439 49.401 67.796 1.00 32.82 6 ATOM 2480 O CYS À 311 33.439 49.401 67.796 1.00 32.82 6 ATOM 2481 N GLU À 312 31.557 43.222 7.08 07 1.00 32.82 6 ATOM 2489 C C CYS À 311 33.499 4.01 67.796 1.00 32.82 6 ATOM 2489 C C CEU À 313 33.515 44.796 7.048 1.00 32.82 6 ATOM 2480 C C SER À 314 33.349 49.401 67.796 1.00 32.82 6 ATOM 2480 C C SER À 314 33.349 49.401 67.796 1.00 32.81 6 ATOM 2495 C C SER À 314 33.349 49.401 67.796 1.00 32. | | | CD2 | LEU A | 308 | | | | | 66 965 | | | 6 |
| ATOM 2455 N LLE A 309 30.1.08 43.017 66.540.1.00 35.78 7 6 ATOM 2454 CA LLE A 309 30.939 41.949 65.431 1.00 34.95 6 6 ATOM 2455 CB LLE A 309 30.939 41.949 65.431 1.00 34.95 6 ATOM 2456 CG2 LLE A 309 30.939 41.949 65.431 1.00 34.95 6 ATOM 2457 CG1 LLE A 309 29.445 41.631 65.212 1.00 34.25 6 ATOM 2458 CD1 LLE A 309 29.445 41.631 65.212 1.00 34.25 6 ATOM 2459 C LLE A 309 32.589 43.238 66.772 1.00 35.81 6 ATOM 2459 C LLE A 309 33.183 42.617 67.657 1.00 35.81 6 ATOM 2461 N TRP A 310 33.197 44.111 65.977 1.00 35.26 6 ATOM 2462 CA TRP A 310 33.197 44.111 65.977 1.00 36.10 7 ATOM 2461 CD TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2465 CD TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.706 46.804 65.380 1.00 30.62 ATOM 2467 CE3 TRP A 310 37.706 46.804 65.380 1.00 30.62 ATOM 2467 CE3 TRP A 310 37.206 46.804 65.380 1.00 30.62 ATOM 2467 CE3 TRP A 310 37.206 46.804 65.380 1.00 30.62 ATOM 2467 CE3 TRP A 310 37.206 46.804 65.380 1.00 29.93 6 ATOM 2467 CE3 TRP A 310 38.852 66.527 41.00 29.93 6 ATOM 2467 CE3 TRP A 310 38.852 66.529 65.336 1.00 29.37 7 ATOM 2467 CE3 TRP A 310 38.852 66.529 65.336 1.00 29.37 7 ATOM 2470 CE2 TRP A 310 38.852 66.529 65.336 1.00 29.37 7 ATOM 2471 CE3 TRP A 310 38.852 66.529 65.336 1.00 29.37 7 ATOM 2471 CE3 TRP A 310 38.852 66.895 1.00 30.62 6 ATOM 2472 CH2 TRP A 310 38.852 66.895 1.00 30.62 7 ATOM 2473 C TRP A 310 38.852 66.895 1.00 30.62 7 ATOM 2471 CE3 TRP A 310 310 38.555 46.659 65.336 1.00 29.37 7 ATOM 2471 CE3 TRP A 310 310 38.555 46.659 65.336 1.00 29.37 7 ATOM 2471 CE3 TRP A 310 310 38.555 46.659 7 1.00 30.62 6 ATOM 2472 CH2 TRP A 310 310 38.555 46.659 7 1.00 30.62 6 ATOM 2473 C TRP A 310 310 38.555 46.659 7 1.00 30.62 6 ATOM 2470 CE2 TRP A 310 310 38.555 46.659 7 1.00 30.62 6 ATOM 2470 CE2 TRP A 310 310 30.62 6 ATOM 2470 CE2 TRP A 310 310 30.62 6 ATOM 2470 CE2 TRP A 310 310 30.62 6 ATOM 2470 CE2 TRP A 310 30.03 | MOTA | | | LEU A | 308 | | | | | 67.975 | 1.00 | 33.75 | 8 |
| ATOM 2455 CB ILE A 309 31. 108 43. 017 66.540 1.00 35.87 6 ATOM 2455 CG ILE A 309 30.939 41.949 65. 431 1.00 34.95 6 ATOM 2456 CG2 ILE A 309 32.945 41.614 65.212 1.00 34.25 6 ATOM 2457 CG1 ILE A 309 28.726 41.014 66.407. 1.00 25.04 6 ATOM 2458 CD1 ILE A 309 32.589 43.238 66.772 1.00 38.19 8 ATOM 2459 C ILE A 309 32.589 43.238 66.772 1.00 35.81 6 ATOM 2460 O ILE A 309 33.183 42.617 67.657 1.00 38.19 8 ATOM 2461 N TRP A 310 33.197 44.111 65.977 1.00 35.26 6 ATOM 2462 CA TRP A 310 35.150 45.311 65.075 1.00 32.61 6 ATOM 2463 CB TRP A 310 35.150 45.311 65.075 1.00 32.61 6 ATOM 2464 CG TRP A 310 36.619 45.588 65.220 1.00 30.79 6 ATOM 2466 CEZ TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CEZ TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2468 CD1 TRP A 310 37.679 46.65 65.80 1.00 30.62 6 ATOM 2468 CD1 TRP A 310 37.264 66.894 65.880 1.00 30.62 7 ATOM 2469 NEI TRP A 310 37.679 44.620 65.801 1.00 30.62 6 ATOM 2470 CZZ TRP A 310 37.314 32.24 65.174 1.00 29.93 6 ATOM 2471 CZZ TRP A 310 37.679 44.620 65.801 1.00 30.62 6 ATOM 2472 CHZ TRP A 310 38.555 46.659 65.536 1.00 29.37 7 ATOM 2473 C TRP A 310 38.555 66.599 65.579 1.00 26.00 6 ATOM 2473 C TRP A 310 38.978 42.585 65.279 1.00 26.00 6 ATOM 2474 CPZ CKYS A 311 34.183 46.213 67.715 1.00 34.57 7 ATOM 2478 C CYS A 311 34.183 46.213 67.715 1.00 34.57 7 ATOM 2478 C CYS A 311 33.169 48.085 68.985 1.00 32.82 6 ATOM 2479 C CYS A 311 33.169 48.085 77.844 1.00 32.82 6 ATOM 2488 C C CLU A 312 33.03 34.940 70.053 1.00 32.52 6 ATOM 2489 O CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C C CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C C CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C C CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C C CYS A 311 33.499 4.001 67.796 1.00 32.306 6 ATOM 2489 C C CYS A 311 33.497 4.009 70.053 1.00 32.701 6 ATOM 2489 C C CYS A 311 33.497 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 70.000 | MOTA | | | LEU A | 308 | | | | | 66.208 | 1.00 | 35.78 | |
| ATOM 2455 CB ILE A 309 30.939 41.949 65.431 1.00 34.95 6 ATOM 2456 CG2 ILE A 309 31.733 40.695 65.799 1.00 31.21 6 ATOM 2457 CG1 ILE A 309 29.445 41.631 65.212 1.00 34.25 6 ATOM 2458 CD1 ILE A 309 29.445 41.631 65.212 1.00 34.25 6 ATOM 2459 C ILE A 309 32.589 43.238 66.772 1.00 35.81 6 ATOM 2469 C ILE A 309 32.589 43.238 66.772 1.00 35.81 6 ATOM 2461 N TRP A 310 33.197 44.111 65.977 1.00 36.10 7 ATOM 2461 N TRP A 310 33.197 44.111 65.977 1.00 35.26 6 ATOM 2462 CA TRP A 310 35.150 45.311 65.075 1.00 32.61 6 ATOM 2463 CB TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.31 43.224 65.174 1.00 31.95 6 ATOM 2466 CE2 TRP A 310 37.31 43.224 65.174 1.00 31.96 6 ATOM 2466 CE2 TRP A 310 37.31 43.224 65.174 1.00 30.62 6 ATOM 2468 CD1 TRP A 310 37.206 46.804 55.380 1.00 30.62 6 ATOM 2468 CD1 TRP A 310 37.206 46.804 55.380 1.00 30.62 6 ATOM 2469 NEI TRP A 310 37.206 46.804 55.380 1.00 30.62 6 ATOM 2467 CE3 TRP A 310 37.31 43.224 65.174 1.00 21.96 6 ATOM 2470 C22 TRP A 310 37.31 43.224 65.174 1.00 21.96 6 ATOM 2471 CZ3 TRP A 310 37.316 44.676 65.99 65.536 1.00 29.37 7 ATOM 2473 C TRP A 310 31.34.34 46.23 67.715 1.00 36.00 6 ATOM 2473 C TRP A 310 35.565 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.565 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2478 S C CYS A 311 33.193 49.401 67.796 1.00 32.01 6 ATOM 2486 C C LEU A 312 33.163 4.474 4.159 71.171 1.00 33.60 6 ATOM 2486 C C LEU A 312 33.163 4.474 4.159 71.171 1.00 33.60 6 ATOM 2487 C CZ CRS A 311 33.912 46.013 71.280 71.00 32.01 6 ATOM 2486 C C LEU A 313 35.913 39.95 67.793 71.00 32.97 8 ATOM 2489 C C LEU A 313 35.565 67.793 71.00 32.00 33.45 7 7 ATOM 2488 C C LEU A 313 35.56 | MOTA | | | ILE A | 309 - | | | | | | 1.00 | 35.87 | |
| ATOM 2455 CGZ IILE A 309 ATOM 2457 CGI IILE A 309 ATOM 2458 CDI IILE A 309 ATOM 2458 CDI IILE A 309 ATOM 2458 CDI IILE A 309 ATOM 2459 CDI IILE A 309 ATOM 2460 O IILE A 309 ATOM 2461 N TRP A 310 ATOM 2461 N TRP A 310 ATOM 2462 CA TRP A 310 ATOM 2463 CB TRP A 310 ATOM 2465 CDZ TRP A 310 ATOM 2466 CEZ TRP A 310 ATOM 2467 CEZ TRP A 310 ATOM 2468 CDI TRP A 310 ATOM 2468 CDI TRP A 310 ATOM 2469 NEI TRP A 310 ATOM 2471 CZZ TRP A 310 ATOM 2471 CZZ TRP A 310 ATOM 2472 CHZ TRP A 310 ATOM 2473 C TRP A 310 ATOM 2474 O TRP A 310 ATOM 2475 N CYS A 311 ATOM 2476 CA CYS A 311 ATOM 2478 SG CYS A 311 ATOM 2479 C CYS A 311 ATOM 2481 N GLU A 312 ATOM 2482 CA GLU A 312 ATOM 2483 C G GLU A 312 ATOM 2485 C GLU A 312 ATOM 2486 C CLU A 312 ATOM 2487 C C GLU A 312 ATOM 2488 C GLU A 312 ATOM 2489 C GLU A 313 ATOM 2489 C GLU A 312 ATOM 2489 C GLU A 313 ATOM 2489 C GLU A 312 ATOM 2489 C GLU A 313 ATOM 2489 C GLU A 312 ATOM 2489 C GLU A 313 ATOM 2499 C C GLU A 312 ATOM 2499 C C GLU A 313 ATOM 2490 C C GLU A 312 ATOM 2490 C C GLU A 312 ATOM 2490 N LEU A 313 ATOM 2490 N LEU A 313 ATOM 2491 C A GLU A 312 ATOM 2490 N LEU A 313 ATOM 2490 N G | | | | ILE A | 309 | | | | | 65.431 | 1.00 | 34.95 | |
| ATOM 2459 CGI ILE A 3099 28,745 41,631 65,212 1.00 34.25 6 ATOM 2459 C ILE A 3099 32,589 43,238 66,772 1.00 35.81 6 ATOM 2460 O ILE A 3099 33,183 42,617 67,657 1.00 35.81 6 ATOM 2461 N TRP A 310 33,197 44.111 65,977 1.00 36.10 7 ATOM 2462 CA TRP A 310 33,197 44.111 65,977 1.00 36.10 7 ATOM 2463 CB TRP A 310 35.150 45.311 65,075 1.00 32.61 6 ATOM 2463 CB TRP A 310 35.150 45.311 65,075 1.00 32.61 6 ATOM 2464 CG TRP A 310 37,679 44.620 65.274 1.00 29.93 6 ATOM 2466 CEZ TRP A 310 37,679 44.620 65.274 1.00 29.93 6 ATOM 2466 CEZ TRP A 310 37,206 46.804 65,380 1.00 30.79 6 ATOM 2466 CEZ TRP A 310 37.206 46.804 65,380 1.00 30.62 7 ATOM 2467 CEZ TRP A 310 38.882 45.330 65.474 1.00 28.42 6 ATOM 2467 CEZ TRP A 310 38.862 65.578 1.00 29.93 6 ATOM 2468 CDI TRP A 310 38.565 46.659 65.536 1.00 29.37 7 ATOM 2467 CEZ TRP A 310 38.882 45.330 65.474 1.00 28.42 6 ATOM 2467 CEZ TRP A 310 38.565 46.699 65.578 1.00 30.62 6 ATOM 2470 CEZ TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2471 CEZ TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2472 CHZ TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2472 CHZ TRP A 310 35.365 46.499 67.715 1.00 36.00 6 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2473 C TRP A 310 35.365 46.476 68.400 1.00 30.62 6 ATOM 2473 C CTRP A 310 34.744 45.000 67.545 1.00 36.00 6 ATOM 2477 CB CYS A 311 34.134 46.213 67.715 1.00 34.57 7 ATOM 2479 C CYS A 311 34.134 46.213 67.715 1.00 34.57 7 ATOM 2479 C CYS A 311 34.134 46.213 7 ATOM 2479 C CYS A 311 34.134 46.213 7 ATOM 2479 C CYS A 311 33.192 46.061 70.206 1.00 32.01 6 ATOM 2479 C CYS A 311 33.192 46.061 70.206 1.00 32.02 6 ATOM 2479 C CYS A 311 33.493 49.401 67.796 1.00 32.35 16 ATOM 2479 C CYS A 311 33.493 49.401 67.796 1.00 32.35 16 ATOM 2480 O CYS A 311 33.157 43.252 70.807 1.00 34.19 6 ATOM 2480 O CYS A 311 33.157 43.252 70.807 1.00 34.19 6 ATOM 2480 O CYS A 311 33.1557 43.252 70.807 1.00 33.455 7 ATOM 2480 O CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2480 O CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2480 O CYS A 311 33.912 46.06 | | | | TLE A | 309 | | | | | | 1.00 | 31.21 | |
| ATOM 2458 CD1 ILE A 309 | | | | ILE A | 309 | 29 | .445 | | | | 1.00 | 34.25 | |
| ATOM 2459 C ILE A 309 33.183 42.617 67.557 1.00 38.19 8 ATOM 2461 N TRP A 310 33.197 44.111 65.977 1.00 36.10 7 ATOM 2462 CA TRP A 310 35.150 45.311 65.977 1.00 35.26 6 ATOM 2463 CB TRP A 310 35.150 45.311 65.075 1.00 32.61 6 ATOM 2464 CG TRP A 310 35.150 45.311 65.075 1.00 32.61 6 ATOM 2465 CD2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.731 43.224 65.174 1.00 31.59 6 ATOM 2468 CD1 TRP A 310 37.731 43.224 65.174 1.00 31.59 6 ATOM 2469 NEI TRP A 310 38.882 45.330 65.344 1.00 29.37 7 ATOM 2469 NEI TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2470 C22 TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2471 C23 TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2472 CHZ TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2474 O TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2475 N CYS A 311 34.134 46.213 67.715 1.00 36.00 6 ATOM 2476 CC CYS A 311 33.169 48.085 68.996 1.00 35.62 6 ATOM 2477 CB CYS A 311 33.199 49.401 67.796 1.00 32.01 6 ATOM 2479 C CYS A 311 33.191 46.061 70.206 1.00 32.01 6 ATOM 2479 C CYS A 311 33.192 46.061 70.206 1.00 32.01 6 ATOM 2480 O CYS A 311 33.193 49.401 67.796 1.00 32.26 16 ATOM 2480 O CYS A 311 33.193 49.401 67.796 1.00 32.277 7 ATOM 2480 CB GLU A 312 33.024 46.031 70.206 1.00 32.07 7 ATOM 2481 N GLU A 312 33.062 45.049 70.053 1.00 32.57 7 ATOM 2482 CA GLU A 312 33.093 42.821 73.239 1.00 43.80 6 ATOM 2487 CE2 GLU A 313 33.13 44.155 70.473 1.00 44.81 8 ATOM 2489 O CUS A 311 33.23 42.604 70.099 1.00 33.49 7 ATOM 2480 CB GLU A 312 30.546 43.527 70.807 1.00 34.19 6 ATOM 2487 CE2 GLU A 313 35.584 42.597 70.093 1.00 32.07 6 ATOM 2488 C GLU A 312 30.642 43.259 70.473 1.00 32.97 6 ATOM 2489 C CB LEU A 313 35.584 42.795 77.1171 1.00 33.65 6 ATOM 2490 C CB SER A 314 38.906 44.064 70.099 1.00 33.49 7 ATOM 2490 C CB SER A 314 38.223 42.957 72.603 1.00 32.97 6 ATOM 2490 C CB SER A 314 38.253 42.957 72.603 1.00 33.49 7 ATOM 2490 C CB SER A 314 38.004 43.253 70.4 | | | | ILE A | 309 | | | | | | | | |
| ATOM 2460 O ILE A 309 ATOM 2461 N TRP A 310 ATOM 2461 N TRP A 310 ATOM 2462 CA TRP A 310 ATOM 2462 CA TRP A 310 ATOM 2463 CB TRP A 310 ATOM 2464 CG TRP A 310 ATOM 2464 CG TRP A 310 ATOM 2465 CD2 TRP A 310 ATOM 2465 CD2 TRP A 310 ATOM 2466 CE2 TRP A 310 ATOM 2466 CE2 TRP A 310 ATOM 2467 CE3 TRP A 310 ATOM 2467 CE3 TRP A 310 ATOM 2468 CD1 TRP A 310 ATOM 2469 NEL TRP A 310 ATOM 2470 CZZ TRP A 310 ATOM 2471 CZZ TRP A 310 ATOM 2472 CHZ TRP A 310 ATOM 2473 C TRP A 310 ATOM 2474 O TRP A 310 ATOM 2475 N CYS A 311 ATOM 2476 CA CYS A 311 ATOM 2476 CA CYS A 311 ATOM 2477 CB CYS A 311 ATOM 2478 SG CYS A 311 ATOM 2479 C C CYS A 311 ATOM 2480 O CYS A 311 ATOM 2480 C C CYS A 311 ATOM 2480 C C CYS A 311 ATOM 2480 C C C C C C C C C C C C C C C C C C C | | | | ILE A | 309 | | | | | | | | |
| ATOM 2462 CA ATOM 2462 CA TRP A 310 34.612 44.84 66.169 1.00 35.26 6 ATOM 2463 CB TRP A 310 35.150 45.311 65.075 1.00 30.79 6 ATOM 2465 CD2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2465 CE2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.679 44.620 65.274 1.00 30.79 6 ATOM 2466 CE2 TRP A 310 37.206 46.804 65.300 65.474 1.00 31.59 6 ATOM 2468 CD1 TRP A 310 37.206 46.804 65.308 1.00 31.59 6 ATOM 2469 NEI TRP A 310 37.206 46.804 65.538 1.00 29.37 7 ATOM 2469 NEI TRP A 310 37.206 46.804 65.538 1.00 29.37 7 ATOM 2479 CZ2 TRP A 310 38.865 46.659 65.536 1.00 29.37 7 ATOM 2471 CZ3 TRP A 310 38.878 42.585 65.279 1.00 28.06 6 ATOM 2471 CZ3 TRP A 310 34.744 45.040 67.545 1.00 36.00 6 ATOM 2473 C TRP A 310 34.744 45.040 67.545 1.00 36.00 6 ATOM 2473 C TRP A 310 34.344 46.213 67.715 1.00 36.00 6 ATOM 2477 CB CYS A 311 34.134 46.213 67.715 1.00 34.57 7 ATOM 2476 CA CYS A 311 34.134 46.213 67.715 1.00 32.82 6 ATOM 2477 C CYS A 311 34.134 46.213 67.715 1.00 32.82 6 ATOM 2477 C CYS A 311 33.169 48.085 68.985 1.00 32.82 6 ATOM 2479 C CYS A 311 33.169 48.085 68.985 1.00 32.82 6 ATOM 2479 C CYS A 311 33.169 48.085 68.985 1.00 32.82 6 ATOM 2480 C CYS A 311 33.494 49.01 67.796 1.00 32.36 16 ATOM 2482 CA GLU A 312 33.062 45.049 70.053 1.00 32.82 6 ATOM 2482 CA GLU A 312 33.062 45.049 70.053 1.00 32.37 6 ATOM 2480 CB GLU A 312 33.062 45.049 70.053 1.00 32.37 6 ATOM 2488 C G GLU A 312 33.932 46.061 70.206 1.00 32.01 6 ATOM 2489 C C GLU A 312 33.933 44.252 70.807 71.171 1.00 33.86 6 ATOM 2489 C C GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2489 C C GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2489 C C GLU A 313 35.584 42.257 70.807 70.00 33.45 7 ATOM 2489 C C GLU A 313 35.584 42.257 70.807 70.00 33.45 7 ATOM 2489 C C GLU A 313 35.584 42.257 70.807 70.00 33.47 6 ATOM 2499 C C SER A 314 33.35.587 39.956 67.269 1.00 33.77 6 ATOM 2499 C C SER A 314 33.35.587 39.956 67.269 1.00 33.77 6 ATOM 2499 C C SER A 314 38.064 46.064 70.099 1.00 33.79 7 ATOM 2499 C C SER A 314 38.107 46.239 70.00 31.00 32.14 6 AT | | | 0 | ILE A | 309 | | | | | | | | |
| ATOM 2463 CB TRP A 310 | | 2461 | N | TRP A | 310 | | | | | | | | 6 |
| ATOM 2464 CG TRP A 310 37.679 44.620 65.274 1.00 30.79 6 ATOM 2465 CD2 TRP A 310 37.679 44.620 65.274 1.00 29.93 6 ATOM 2466 CE2 TRP A 310 37.679 44.620 65.274 1.00 28.42 6 ATOM 2467 CE3 TRP A 310 37.731 43.224 65.174 1.00 31.59 6 ATOM 2468 CD1 TRP A 310 37.731 43.224 65.174 1.00 31.59 6 ATOM 2469 NEI TRP A 310 38.565 46.659 65.536 1.00 29.37 7 ATOM 2469 NEI TRP A 310 38.565 46.659 65.536 1.00 27.91 6 ATOM 2470 CZ2 TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2471 CZ3 TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2471 CZ3 TRP A 310 35.365 44.476 68.440 1.00 36.00 6 ATOM 2472 CH2 TRP A 310 35.365 44.476 68.440 1.00 36.00 6 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2474 O TRP A 310 34.183 46.937 68.985 1.00 32.32 6 ATOM 2475 N CYS A 311 34.183 46.937 68.985 1.00 32.32 6 ATOM 2476 CA CYS A 311 33.169 48.085 68.995 1.00 32.36 16 ATOM 2477 CB CYS A 311 33.39 49.401 67.796 1.00 32.36 16 ATOM 2478 CG CYS A 311 33.49 49.401 67.796 1.00 32.36 16 ATOM 2478 C CYS A 311 33.49 49.401 67.796 1.00 32.36 16 ATOM 2480 C CYS A 311 33.492 49.401 67.796 1.00 32.35 16 ATOM 2480 C CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2480 C CYS A 311 33.052 45.049 70.053 1.00 32.37 7 ATOM 2481 N GLU A 312 33.052 45.049 70.053 1.00 32.37 7 ATOM 2482 CA GLU A 312 31.557 43.252 70.807 1.00 34.57 7 ATOM 2488 C G GLU A 312 31.557 43.252 70.807 1.00 34.57 7 ATOM 2488 C G GLU A 312 31.557 43.252 70.807 1.00 34.19 6 ATOM 2489 C D GLU A 312 31.685 41.831 73.383 1.00 44.8 8 ATOM 2489 C D GLU A 313 35.584 2.251 73.299 1.00 43.80 6 ATOM 2490 N LEU A 313 35.584 2.251 73.299 1.00 43.80 6 ATOM 2491 CA LEU A 313 35.584 42.252 70.807 1.00 33.45 7 ATOM 2492 CB LEU A 313 35.584 42.253 70.473 1.00 32.97 8 ATOM 2493 C G LEU A 313 35.584 42.253 70.473 1.00 32.14 6 ATOM 2495 C C LEU A 313 35.595 40.093 1.00 32.07 8 ATOM 2496 C LEU A 313 35.595 40.493 70.903 1.00 31.40 6 ATOM 2497 O LEU A 313 35.596 43.295 70.473 1.00 37.82 6 ATOM 2498 N SER A 314 39.414 47.120 69.353 1.00 37.42 8 ATOM 2499 C SER A 314 39.414 47.120 69.353 1.00 34.45 8 | | _ | | TRP A | 310 | | | | | | 1.00 | 32.61 | |
| ATOM 2465 CD2 TRP A 310 | ATOM | | | TRP A | 310 | | | | | | 1.00 | 30.79 | |
| ATOM 2466 CE2 TRP A 310 ATOM 2466 CE2 TRP A 310 ATOM 2467 CE3 TRP A 310 ATOM 2468 CD1 TRP A 310 ATOM 2468 CD1 TRP A 310 ATOM 2469 NE1 TRP A 310 ATOM 2470 CZ2 TRP A 310 ATOM 2470 CZ2 TRP A 310 ATOM 2471 CZ3 TRP A 310 ATOM 2471 CZ3 TRP A 310 ATOM 2471 CZ3 TRP A 310 ATOM 2472 CH2 TRP A 310 ATOM 2473 C TRP A 310 ATOM 2474 O TRP A 310 ATOM 2475 N CYS A 311 ATOM 2476 CA CYS A 311 ATOM 2476 CA CYS A 311 ATOM 2477 CB CYS A 311 ATOM 2477 CB CYS A 311 ATOM 2477 CB CYS A 311 ATOM 2478 CG CYS A 311 ATOM 2479 C CYS A 311 ATOM 2479 C CYS A 311 ATOM 2480 O CYS A 311 ATOM 2481 N GUU A 312 ATOM 2482 CA GLU A 312 ATOM 2482 CA GLU A 312 ATOM 2485 CD GLU A 312 ATOM 2486 CB GLU A 312 ATOM 2487 CG GLU A 312 ATOM 2488 C GLU A 312 ATOM 2488 C GLU A 312 ATOM 2488 C GLU A 312 ATOM 2489 O GLU A 312 ATOM 2489 CA GLU A 313 ATOM 2489 CA GLU A 31 | | | | TRP A | 310 | | | | | | 1.00 | 29.93 | |
| ATOM 2467 CE3 TRP A 310 | | | | מ מסת | 310 | | | | | | 1.00 | 28.42 | |
| ATOM 2468 CD1 TRP A 310 | | | | | | | | | 43.224 | | | | |
| ATOM 2469 NE1 TRP A 310 38.565 46.659 65.578 1.00 27.91 6 ATOM 2471 CZ3 TRP A 310 38.978 42.585 65.279 1.00 28.06 6 ATOM 2471 CZ3 TRP A 310 40.126 44.691 65.578 1.00 36.00 6 ATOM 2472 CH2 TRP A 310 40.150 43.322 65.479 1.00 36.00 6 ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.00 6 ATOM 2474 O TRP A 310 35.365 44.476 68.440 1.00 36.24 ATOM 2475 N CYS A 311 34.183 46.233 67.715 1.00 34.57 7 ATOM 2476 CA CYS A 311 33.4183 46.233 68.985 1.00 32.82 6 ATOM 2477 CB CYS A 311 33.4183 46.937 68.985 1.00 32.82 6 ATOM 2478 SG CYS A 311 33.4193 49.401 67.796 1.00 32.36 16 ATOM 2479 C CYS A 311 33.912 46.061 70.206 1.00 32.01 ATOM 2479 C CYS A 311 33.912 46.061 70.206 1.00 32.01 ATOM 2480 O CYS A 311 33.062 45.049 70.053 1.00 32.57 7 ATOM 2481 N GLU A 312 33.062 45.049 70.053 1.00 32.57 7 ATOM 2482 CA GLU A 312 32.731 44.159 71.171 1.00 33.86 6 ATOM 2483 CB GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.516 43.522 74.195 1.00 34.80 6 ATOM 2488 C GLU A 312 30.516 43.522 74.195 1.00 32.07 8 ATOM 2490 N LEU A 313 35.687 42.995 77.2603 1.00 32.07 8 ATOM 2490 N LEU A 313 35.587 39.956 67.269 1.00 33.45 7 ATOM 2490 N LEU A 313 35.584 42.135 70.473 1.00 32.89 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 7 ATOM 2499 CA SER A 314 38.107 40.493 68.626 1.00 27.737 6 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.787 6 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2499 CA SER A 314 38.046 45.661 71.730 1.00 33.65 7 ATOM 2499 CA SER A 314 38.046 45.661 71.730 1.00 33.65 7 | | | | | | 3 | 7.206 | | | | 1.00 | 30.64 | |
| ATOM 2470 CZ2 TRP A 310 | | | | | 310 | | | | | | | | |
| ATOM 2471 C23 TRP A 310 | | | | TRP A | A 310 | | | | | | | | |
| ATOM 2473 C TRP A 310 | | 2471 | CZ3 | TRP A | 4 310 | | | | | | | | |
| ATOM 2473 C TRP A 310 35.365 44.476 68.440 1.00 36.24 8 ATOM 2475 N CYS A 311 34.134 46.213 67.715 1.00 34.57 7 ATOM 2476 CA CYS A 311 34.183 46.937 68.996 1.00 32.82 6 ATOM 2477 CB CYS A 311 33.199 48.085 68.996 1.00 32.82 6 ATOM 2478 SG CYS A 311 33.199 49.401 67.796 1.00 32.36 16 ATOM 2479 C CYS A 311 33.419 49.401 67.796 1.00 32.01 6 ATOM 2480 O CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2481 N GLU A 312 33.062 45.049 70.053 1.00 32.57 7 ATOM 2482 CA GLU A 312 32.731 44.159 71.171 1.00 33.86 6 ATOM 2483 CB GLU A 312 31.557 43.252 70.807 1.00 34.19 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2486 OE1 GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2488 C GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2489 O GLU A 312 30.933 42.821 73.239 1.00 43.80 6 ATOM 2489 O GLU A 312 30.516 43.522 74.195 1.00 31.77 6 ATOM 2489 O GLU A 313 33.647 42.945 70.382 1.00 32.07 8 ATOM 2490 N LEU A 313 36.647 42.945 70.382 1.00 32.07 8 ATOM 2491 CA LEU A 313 35.584 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2493 CG LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2496 C LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2497 O LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2498 N SER A 314 33.067 44.064 70.099 1.00 31.74 8 ATOM 2499 CA SER A 314 38.074 40.647 70.388 1.00 44.55 8 ATOM 2499 CA SER A 314 38.074 40.656 70.388 1.00 37.32 6 ATOM 2490 N GLY A 315 36.976 43.031 70.993 1.00 37.32 6 ATOM 2490 N GLY A 315 36.906 46.243 73.498 1.00 44.55 8 ATOM 2500 CB SER A 314 39.015 46.043 72.395 1.00 37.32 6 ATOM 2501 OG SER A 314 39.015 46.043 72.395 1.00 37.32 6 ATOM 2502 C SER A 314 39.015 46.043 72.395 1.00 37.32 6 ATOM 2506 C GLY A 315 36.596 47.744 73.568 1.00 46.80 6 | | 2472 | CH2 | TRP A | A 310 | | | | | | | | 6 |
| ATOM 2476 CA CYS A 311 34.134 46.213 67.715 1.00 34.57 7 ATOM 2476 CA CYS A 311 34.183 46.937 68.985 1.00 32.82 6 ATOM 2477 CB CYS A 311 33.169 48.085 68.985 1.00 32.82 6 ATOM 2478 SG CYS A 311 33.169 48.085 68.996 1.00 32.36 16 ATOM 2479 C CYS A 311 33.194 46.061 70.206 1.00 32.01 6 ATOM 2479 C CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2480 O CYS A 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2481 N GLU A 312 33.062 45.049 70.053 1.00 32.57 7 ATOM 2481 N GLU A 312 32.731 44.159 71.171 1.00 33.86 6 ATOM 2482 CA GLU A 312 31.557 43.252 70.807 1.00 34.19 6 ATOM 2483 CB GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 44.81 8 ATOM 2486 OEI GLU A 312 30.923 42.821 73.338 1.00 44.81 8 ATOM 2488 C GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2489 O GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2489 O GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2491 CA LEU A 313 36.172 41.513 69.15 1.00 32.07 6 ATOM 2492 CB LEU A 313 36.172 41.513 69.15 1.00 32.14 6 ATOM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 37.73 6 ATOM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 37.73 6 ATOM 2499 CD LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2499 CD LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2499 CD LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2499 CD LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2499 CD LEU A 313 35.053 39.367 69.648 1.00 27.73 6 ATOM 2499 CD LEU A 313 35.053 39.367 69.648 1.00 27.73 6 ATOM 2499 CD LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2499 CD SER A 314 38.204 45.661 71.730 1.00 32.14 6 ATOM 2499 CD SER A 314 38.107 46.6154 69.256 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.32 8 A | MOTA | | | TRP A | A 310 | | | | | _ | 1.00 | | |
| ATOM 2476 CA CYS A 311 33.169 48.085 68.985 1.00 32.36 6 6 1 | | | | TRP | A 310 | | | | | | | | |
| ATOM 2478 GC CYS A 311 | | | | CYS | A 311 | | | | | | 1.00 | 32.82 | |
| ATOM 2478 SG CYS À 311 33.439 49.401 67.796 1.00 32.01 6 ATOM 2479 C CYS À 311 33.912 46.061 70.206 1.00 32.01 6 ATOM 2480 O CYS À 311 34.452 46.313 71.280 1.00 29.82 8 ATOM 2481 N GLU À 312 33.062 45.049 70.053 1.00 32.57 7 ATOM 2482 CÀ GLU À 312 32.731 44.159 71.171 1.00 33.86 6 ATOM 2483 CB GLU À 312 30.442 43.185 71.844 1.00 40.27 6 ATOM 2485 CD GLU À 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2486 OEI GLU À 312 30.923 42.821 73.383 1.00 44.81 8 ATOM 2486 OEI GLU À 312 30.516 43.522 74.195 1.00 31.77 6 ATOM 2488 C GLU À 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2489 O GLU À 312 34.253 42.957 72.603 1.00 32.07 8 ATOM 2490 N LEU À 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2491 CÀ LEU À 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU À 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2493 CG LEU À 313 35.587 39.367 69.648 1.00 27.73 6 ATOM 2494 CD1 LEU À 313 35.587 39.566 67.269 1.00 30.39 6 ATOM 2496 C LEU À 313 35.053 39.367 69.648 1.00 27.73 6 ATOM 2497 O LEU À 313 35.053 39.367 69.648 1.00 27.73 6 ATOM 2498 N SER À 314 38.232 45.067 70.328 1.00 31.64 6 ATOM 2497 O LEU À 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2498 N SER À 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2498 N SER À 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2498 N SER À 314 38.232 45.067 70.328 1.00 37.82 6 ATOM 2499 CA SER À 314 38.232 45.067 70.328 1.00 37.82 6 ATOM 2499 CA SER À 314 38.232 45.067 70.328 1.00 37.82 6 ATOM 2500 CB SER À 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER À 314 39.114 47.120 69.353 1.00 44.55 8 ATOM 2500 CB SER À 314 39.114 47.120 69.353 1.00 37.32 6 ATOM 2500 CB SER À 314 39.015 46.043 72.395 1.00 37.32 6 ATOM 2500 CB SER À 314 39.015 46.043 72.395 1.00 37.32 6 ATOM 2500 CB SER À 314 39.015 46.043 73.568 1.00 46.80 6 ATOM 2500 CB SER À 314 39.015 46.043 73.3568 1.00 46.80 6 ATOM 2500 CB SER À 314 39.015 46.043 73.3568 1.00 46.80 6 ATOM 2500 CB SER À 314 39.015 46.043 73.3568 1.00 46.80 6 ATOM 2500 CB SER À 314 39.015 46.043 73.3568 1.00 46.80 6 ATOM 2500 CB SER À 314 39.015 46.043 73.568 1.00 46.80 6 | | _ | | | | | | | 48.085 | | 1.00 | 35.62 | |
| ATOM 2480 O CYS A 311 | | | | | | 3 | 3.439 | | | | 1.00 | 32.30 | |
| ATOM 2480 O CYS A 311 | | _ | | CYS | A 311 | | | - | | | 1.00 | 29 82 | |
| ATOM 2481 N GLU A 312 33.062 45.049 70.033.86 6 ATOM 2482 CA GLU A 312 32.731 44.159 71.171 1.00 33.86 6 ATOM 2483 CB GLU A 312 30.442 43.185 71.844 1.00 40.27 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2486 OE1 GLU A 312 30.923 42.821 73.383 1.00 44.81 8 ATOM 2487 CE2 GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2488 C GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2489 O GLU A 312 34.253 42.957 72.603 1.00 32.07 8 ATOM 2490 N LEU A 313 34.647 42.945 70.328 1.00 33.45 7 ATOM 2491 CA LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2494 CD1 LEU A 313 35.557 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.557 39.956 67.269 1.00 30.39 6 ATOM 2496 C LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2497 N SER A 314 38.232 45.067 70.328 1.00 31.64 6 ATOM 2497 O LEU A 313 37.005 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2499 CA SER A 314 38.207 46.154 69.256 1.00 35.59 6 ATOM 2497 CO LEU A 313 37.006 44.064 70.099 1.00 33.49 7 ATOM 2498 N SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2499 CA SER A 314 38.206 45.661 71.730 1.00 37.32 8 ATOM 2500 CB SER A 314 38.206 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 6 ATOM 2500 N GLY A 315 36.590 47.744 73.568 1.00 47.85 8 | | | | CYS | A 311 | | | - | | | | | |
| ATOM 2483 CB GLU A 312 31.557 43.252 70.807 1.00 34.19 6 ATOM 2484 CG GLU A 312 30.442 43.185 71.844 1.00 40.27 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2486 OE1 GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2487 CE2 GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2488 C GLU A 312 30.516 43.522 74.195 1.00 33.77 6 ATOM 2489 O GLU A 312 34.253 42.957 72.603 1.00 32.07 8 ATOM 2490 N LEU A 313 35.848 42.135 70.382 1.00 33.45 7 ATOM 2491 CA LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2497 O LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 33.49 7 ATOM 2500 CB SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 37.82 6 ATOM 2500 CB SER A 314 38.066 45.661 71.730 1.00 37.82 6 ATOM 2500 C SER A 314 38.066 45.661 71.730 1.00 37.82 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 38.05 7 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 44.55 8 ATOM 2500 C SER A 314 38.046 45.661 71.730 1.00 44.55 8 ATOM 2500 | | 2481 | N | GLU . | A 312 | | | _ | - | | 1.00 | 33.86 | |
| ATOM 2484 CG GLU A 312 30.442 43.185 71.844 1.00 40.27 6 ATOM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATOM 2486 OE1 GLU A 312 30.923 42.821 73.383 1.00 44.81 8 ATOM 2487 OE2 GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2488 C GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATOM 2489 O GLU A 312 34.253 42.957 72.603 1.00 32.07 8 ATOM 2489 O GLU A 313 34.647 42.945 70.382 1.00 33.45 7 ATOM 2490 N LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2493 CG LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2494 CD1 LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2495 CD2 LEU A 313 35.5587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2499 CA SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2499 CA SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 37.82 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37 | | | | GLU | A 312 | | | | | | 1.00 | 34.19 | |
| ATCM 2485 CD GLU A 312 30.923 42.821 73.239 1.00 43.80 6 ATCM 2486 OE1 GLU A 312 31.685 41.831 73.383 1.00 44.81 8 ATOM 2487 CE2 GLU A 312 30.516 43.522 74.195 1.00 41.54 8 ATOM 2488 C GLU A 312 33.953 43.298 71.456 1.00 33.77 6 ATCM 2489 O GLU A 312 34.253 42.957 72.603 1.00 32.07 8 ATCM 2490 N LEU A 313 34.647 42.945 70.382 1.00 33.45 7 ATCM 2491 CA LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATCM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATCM 2493 CG LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATCM 2494 CD1 LEU A 313 35.154 40.493 68.626 1.00 27.87 6 ATCM 2496 C LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATCM 2496 C LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATCM 2497 O LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATCM 2498 N SER A 314 37.605 42.793 71.925 1.00 31.74 8 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 33.49 7 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATCM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATCM 2500 C SER A 314 38.107 46.154 69.256 1.00 37.82 6 ATCM 2500 C SER A 314 38.107 46.154 69.256 1.00 37.82 6 ATCM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATCM 2500 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATCM 2500 C GLY A 315 36.506 46.243 73.498 1.00 44.55 8 ATCM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATCM 2500 C GLY A 315 36.5924 48.438 72.458 1.00 48.90 7 | ATOM | | | GLU | A 314 | | | | | | | | |
| ATOM 2486 OE1 GLU A 312 | | | | CIII | A 312 | | | | | 73.239 | 1.00 | 43.80 | |
| ATOM 2487 CE2 GLU A 312 30.516 43.522 74.195 1.00 41.54 6 | | | | 1 GLU | A 312 | | | | | | 1.00 | 44.81 | |
| ATOM 2488 C GLU A 312 33.953 43.298 71.436 1.00 32.07 8 ATOM 2489 O GLU A 312 34.257 72.603 1.00 32.07 8 ATOM 2490 N LEU A 313 34.647 42.945 70.382 1.00 33.45 7 ATOM 2491 CA LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2492 CB LEU A 313 36.172 41.513 69.115 1.00 32.14 6 ATOM 2493 CG LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 37.32 8 ATOM 2500 CB SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2500 C SER A 314 39.015 46.043 72.395 1.00 37.82 6 ATOM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2500 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2500 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | 2 GLU | A 312 | | 30.516 | 6 | 43.522 | | 1.00 | 41.54 | |
| ATOM 2489 O GLU A 312 34.253 42.957 72.803 1.00 33.45 7 ATOM 2490 N LEU A 313 35.848 42.135 70.473 1.00 32.89 6 ATOM 2491 CA LEU A 313 35.848 42.135 70.473 1.00 32.14 6 ATOM 2492 CB LEU A 313 36.172 41.513 69.115 1.00 32.14 6 ATOM 2493 CG LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2500 CB SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2504 N GLY A 315 36.506 46.243 73.498 1.00 44.55 8 ATOM 2504 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2507 O GLY A 315 36.5923 48.276 74.618 1.00 47.85 8 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | | | | 33.953 | 3 | | 71.456 | | 33.// | |
| ATOM 2490 N LEU A 313 | | | | GLU | A 312 | | | | | | | 32.07 | |
| ATCM 2491 CA LEU A 313 35.848 41.513 69.115 1.00 32.14 6 ATCM 2492 CB LEU A 313 36.172 41.513 69.115 1.00 32.14 6 ATCM 2493 CG LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATCM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATCM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATCM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATCM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATCM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATCM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATCM 2500 CB SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2502 C SER A 314 39.141 47.120 69.353 1.00 37.82 6 ATCM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2507 O GLY A 315 36.596 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 36.295 47.744 73.568 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | N | LEU | A 313 | | 34.64 | 7 | | | | 32.89 | |
| ATOM 2492 CB LEU A 313 35.154 40.493 68.626 1.00 27.73 6 ATOM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATOM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2500 CB SER A 314 39.141 47.120 69.353 1.00 44.55 ATOM 2502 C SER A 314 39.141 47.120 69.353 1.00 37.82 6 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2505 CA GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2507 O GLY A 315 36.595 47.744 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 36.595 47.744 73.568 1.00 47.85 8 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | 2491 | CA | LEU | A 313 | | | | | | | 32.14 | |
| ATCM 2494 CD1 LEU A 313 35.587 39.956 67.269 1.00 30.39 6 ATCM 2495 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATCM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATCM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATCM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATCM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATCM 2500 CB SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2502 C SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2507 O GLY A 315 36.595 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 36.295 47.744 73.568 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | | | | 35 15 | 2 A | | | . 1.00 | 27.73 | 6 |
| ATOM 2494 CD2 LEU A 313 35.053 39.367 69.648 1.00 27.87 6 ATOM 2496 C LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2502 C SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2507 O GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | ATCM | | | LEU | A 313 | | | | | 67.269 | .1.00 | 30.39 | 6 |
| ATOM 2495 CD LEU A 313 36.976 43.031 70.903 1.00 31.64 6 ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.49 7 ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2502 C SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 O SER A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2507 O GLY A 315 36.595 47.744 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | | Y 212 | | | | | 69.648 | 1.00 | 27.87 | 6 |
| ATOM 2497 O LEU A 313 37.605 42.793 71.925 1.00 31.74 8 ATOM 2498 N SER A 314 37.206 44.064 70.099 1.00 33.499 7 ATCM 2498 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2502 C SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATCM 2503 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2503 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.506 46.243 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 48.90 7 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 | | | | 121 | A 313 | | | | | 70.903 | 1.00 | 31.64 | 6 |
| ATCM 2498 N SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATCM 2499 CA SER A 314 38.232 45.067 70.328 1.00 35.59 6 ATCM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATCM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATCM 2502 C SER A 314 39.141 47.120 69.353 1.00 37.82 6 ATCM 2503 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2507 O GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | LEU | A 313 | | | | | | | 31.74 | 7 |
| ATOM 2499 CA SER A 314 38.232 45.067 70.328 1.00 36.47 6 ATOM 2500 CB SER A 314 38.107 46.154 69.256 1.00 36.47 6 ATOM 2501 OG SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2502 C SER A 314 38.046 45.661 71.730 1.00 37.82 6 ATOM 2503 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.506 46.243 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | SER | A 314 | | | | | | |) 33.49 | 6 |
| ATOM 2500 CB SER A 314 39.141 47.120 69.353 1.00 44.55 8 ATOM 2501 OG SER A 314 39.141 47.120 69.353 1.00 37.82 6 ATOM 2502 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATOM 2503 C SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATOM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | | A 314 | | 38.23 | 2 | | | | 36 17 | |
| ATCM 2501 OG SER A 314 39.141 47.120 69.333 1.00 37.82 6 ATCM 2502 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATCM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | | A 314 | | | | | | | 1 44 55 | 8 |
| ATCM 2502 C SER A 314 38.046 45.661 71.730 1.00 37.32 8 ATCM 2503 O SER A 314 39.015 46.043 72.395 1.00 37.32 8 ATCM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | SER | A 314 | | | | | | | 37.82 | 6 |
| ATOM 2503 0 SER A 314 39.015 46.045 72.175 1.00 38.05 7 ATOM 2504 N GLY A 315 36.794 45.725 72.175 1.00 38.05 7 ATOM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATOM 2506 C GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATOM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATOM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | SER | A 314 | | | | | | | 37.32 | 8 |
| ATCM 2504 N GLY A 315 36.794 45.723 73.498 1.00 42.42 6 ATCM 2505 CA GLY A 315 36.506 46.243 73.498 1.00 42.42 6 ATCM 2506 C GLY A 315 36.295 47.744 73.568 1.00 46.80 6 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | | | SER | A 314 | | | | | | | 38.05 | 7 |
| ATCM 2505 CA GLY A 315 36.306 48.243 73.568 1.00 46.80 6 ATCM 2506 C GLY A 315 36.295 47.744 73.568 1.00 47.85 8 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | 2504 | 1 N | GLY | A 315 | | | | | | 3 1.0 | 0 42.42 | 6 |
| ATCM 2506 C GLY A 315 35.923 48.276 74.618 1.00 47.85 8 ATCM 2507 O GLY A 315 35.923 48.276 74.618 1.00 48.90 7 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 7 | | 2505 | | GLY | A 315 | | | | | | 1.0 | 0 46.80 | 6 |
| ATCM 2507 O GLY A 313 35.518 48.438 72.458 1.00 48.90 7 ATCM 2508 N ARG A 316 36.518 48.438 72.458 1.00 48.90 | | 2500 | | GLY | Y 312 | | | | | | 1.0 | 0 47.85 | . 8 |
| ATCM 2508 N ARG A 525 | ATCM | 250 | | GLY | A 316 | | | | | | _ | 0 48.90 | 7 |
| | ATCM | 250 | R N | | 7. | | | _ | | - | | | |

| | | | - 50 3 31 | 6 | 36 | 346 | 49.885 | 72.448 | 1.00 52.27 | 6 |
|--------------|--------------|----------|-----------|------------|-----|-------|----------|----------|------------|--------|
| MOTA | 2509 | CA | ARG A 31 | | | 144 | 50.479 | 71.283 | 1.00 53.60 | 6 |
| MOTA | 2510 | CB | ARG A 31 | .0 | | 730 | 50.007 | 69.900 | 1.00 52.11 | 6 |
| ATOM | 2511 | CG | ARG A 31 | .6 | | | 50.514 | 68.870 | 1.00 53.76 | 6 |
| ATOM | 2512 | CD | ARG A 31 | .6 | | 734 | | 69.019 | 1.00 53.67 | 7 |
| MOTA | 2513 | NE | ARG A 31 | .6 | | 028 | 49.854 | 68.383 | 1.00 55.34 | 6 |
| ATOM . | 2514 | CZ | ARG A 31 | .6 | | 135 | 50.221 | 67.552 | 1.00 55.44 | 7 |
| ATOM | 2515 | NH1 | ARG A 31 | .6 | | 110 | 51.253 | | 1.00 55.80 | 7 . |
| ATOM | 2516 | NH2 | ARG A 31 | L 6 | | 266 | 49.546 | 68.569 | 1.00 52.06 | 6 |
| ATOM | 2517 | С | ARG A 31 | 16 | 34. | 882 | 50.343 | 72.391 | | 8 |
| ATOM | 2518 | ō | ARG A 31 | 16 | 34. | 075 | 49.781 | . — | 1.00 54.96 | 7 |
| ATOM | 2519. | N | GLU A 31 | L7 | 34. | 547 | 51.361 | 73.182 | 1.00 51.87 | |
| | 2520 | CA | GLU A.31 | L7 | | 185 | 51.900 | 73.222 | 1.00 52.67 | 6 |
| MOTA | 2521 | CB | GLU A 31 | 17 | 33. | 111 | 53.139 | 74.123 | 1.00 54.70 | 6 |
| MOTA | 2522 | CG | GLU A 31 | 17 | 32. | . 549 | 52.901 | 75.527 | 1.00 60.94 | 6 |
| MOTA | 2523 | CD | GLU A 3 | | | . 353 | 51.912 | 76.361 | 1.00 64.62 | 6 |
| MOTA | 2524 | OE1 | GLU A 3 | | 33. | . 025 | 51.741 | 77.556 | 1.00 64.59 | 8 - |
| ATOM | 2525 | OE2 | <u> </u> | | 34. | . 305 | 51.302 | 75.832 | 1.00 68.64 | 8 |
| ATOM | 2526 | C | GLU A 3 | | 32 | .642 | 52.256 | 71.843 | 1.00 51.27 | 6 |
| MOTA | | Ö | GLU A 3 | | | .270 | 52.983 | 71.077 | 1.00 49.34 | 8 |
| MOTA | 2527 | И | VAL A 3 | | 31 | .457 | 51.733 | 71.548 | 1.00 51.30 | 7 |
| ATOM | 2528 | CA | VAL A 3 | 18 | | .780 | 51.962 | 70.280 | 1.00 48.80 | 6 |
| MOTA | 2529 | | VAL A 3 | | | .522 | 51.071 | 70.169 | 1.00 47.11 | 6 |
| MOTA | 2530 | CB | VAL A 3 | 18 | | .875 | 51.237 | 68.808 | 1.00 45.53 | 6 |
| ATOM | 2531 | CGI | VAL A 3 | 18 | | .895 | 49.631 | 70.424 | 1.00 47.05 | 6 |
| MOTA | 2532 | | VAL A 3 | 10 | | .349 | 53.411 | 70.178 | 1.00 47.64 | 6 |
| MOTA | 2533 | C | VAL A 3 | | | .511 | 53.867 | 70.953 | 1.00 47.61 | 8 |
| ATOM | 2534 | 0 | PRO A 3 | | | .925 | 54.165 | 69.234 | 1.00 48.14 | 7 |
| ATOM | 2535 | N | PRO A 3 | | | .960 | 53.836 | 68.247 | 1.00 48.87 | б |
| MOTA | 2536 | CD | PRO A 3 | | | .538 | 55.569 | 69.093 | 1.00 52.54 | 6 |
| MOTA | 2537 | CA | PRO A 3 | 10 | | .438 | 56.051 | 67.954 | 1.00 49.96 | 6 |
| MOTA | 2538 | CB | PRO A 3 | 10 | | .612 | 54.802 | 67.141 | 1.00 50.17 | 6 |
| MOTA | 2539 | CG | PRO A 3 | | | .052 | 55.679 | 68.764 | 1.00 55.84 | 6 |
| MOTA | 2540 | C | PRO A 3 | | | .531 | 54.913 | 67.953 | 1.00 56.06 | 8 |
| MOTA | 2541 | 0 | GLU A 3 | 20 | | .369 | 56.624 | 69.402 | 1.00 59.20 | 7 |
| MOTA | 2542 | N | GLU A 3 | 20 | | .942 | 56.804 | 69.167 | 1.00 62.61 | 6 |
| MOTA | 2543 | CA | GLU A 3 | 20 | | .302 | 57.588 | 70.313 | 1.00 65.59 | 6 |
| ATOM | 2544 | CB | GLU A 3 | 20 | | .727 | 59.042 | 70.365 | 1.00 73.01 | 6 |
| MOTA | 2545 | CG CD | GLU A 3 | 20 | | .007 | 59.823 | 71.451 | 1.00 76.93 | 6 |
| ATOM | 2546 | OE: | | | | .755 | 59.832 | 71.446 | 1.00 77.37 | 8 |
| MOTA | 2547 2548 | OE. | GLU A 3 | 20 | | .697 | 60.431 | 72.303 | 1.00 79.46 | 8 |
| ATOM | 2549 | C C | GLU A 3 | 320 | 26 | .698 | 57.551 | 67.863 | 1.00 61.40 | 6 |
| ATOM | 2550 | 0 | GLU A 3 | 320 | 25 | .663 | 58.197 | 67.699 | 1.00 62.33 | 8 |
| MOTA | 2551 | Ŋ | LYS A 3 | 321 | 27 | .650 | 57.463 | 66.939 | 1.00 59.47 | 7 |
| ATOM | 2552 | CA | LYS A | 321 | 27 | 7.519 | 58.150 | | 1.00 59.54 | 6 |
| ATOM | 2553 | CB | LYS A 3 | 321 | 27 | 7.340 | 59.648 | | 1.00 61.36 | 6 6 |
| ATOM | 2554 | CG | | | 27 | 3.620 | 60.323 | 66.366 | 1.00 65.23 | 6 |
| MOTA MOTA | 2555 | ÇD | LYS A 3 | 321 | : 3 | .169 | 59.691 | 67.643 | 1.00 66.59 | 6 |
| MOTA | 2556 | CE | LYS A | 321 | | .564 | 60.215 | | 1.00 67.34 | 7 |
| MOTA | 2557 | NZ | LYS A 3 | 321 | 30 |).591 | 61.699 | | 1.00 68.58 | 6 |
| ATOM | 2558 | C | LYS A | 321 | | 3.766 | | | 1.00 59.24 | 8 |
| MOTA | 2559 | ō | LYS A | 321 | | 845 | | | | |
| ATOM | 2560 | N | LEU A | 322 | | 3.608 | | | 1.00 57.55 | 6 |
| ATOM | 2561 | CA | | | 29 | 9.702 | 58.002 | | 1.00 54.72 | |
| | 2562 | CB | | | 29 | 9.171 | | | | 6 |
| ATOM | 2563 | CG | | | 21 | B.141 | 56.316 | | | |
| MOTA | 2564 | CD | 1 LEU A | 322 | | 7.708 | | | | |
| ATOM | 2565 | מה | 2 LEU A | 322 | | 8.716 | | | | |
| MOTA | 2566 | | LEU A | 322 | 3 | 0.250 | 59.406 | 62.313 | | |
| ATOM | 2567 | | LEU A | 322 | 2 | 9.512 | | | | 8 |
| MOTA | 2568 | | ASN A | 323 | | 1.530 | | | | |
| ATOM | 2569 | | | 323 | 3 | 2.089 | | | | |
| ATOM | 2570 | | | 323 | 3 | 3.591 | L 60.90 | | | |
| ATOM | | _ | | 323 | 3 | 4.428 | 3 59.964 | 4 61.189 | | |
| MOTA | 2571 2572 | | 1 ASN A | 323 | | 4.386 | 5 58.744 | | | |
| ATCM | 2573 | | 2 ASN A | 323 | | 5.195 | 60.53 | | | • |
| ATCM | 2574 2574 | | ASN A | 323 | | 1.843 | | 9 60.243 | 1.00 48.63 | , , |
| ATOM | 20/4 | | | | | | | - | | |

| | | | | Figure 1/-40 | | | | |
|--------------|--------------|----------|------------------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 2575 | 0 | ASN A 323 | 31.135 | 60.479 | 59.538 | 1.00 47.52 | 8 |
| ATOM | 2576 | N | ASN A 324 | 32.426 | 62.304 | 59.792 | 1.00 47.66 | 7 |
| ATOM | 2577 | CA | ASN A 324 | 32.242 | 62.769 | 58.419 | 1.00 49.25 | 6 |
| ATOM | 2578 | CB | ASN A 324 | 32.758 | 64.200 | 58.292 | 1.00 50.73 | 6 |
| ATOM | 2579 | CG | ASN A 324 | 32.025 | 65.154 | 59.205 | 1.00 53.83 | 6 |
| ATOM | 2580 | | ASN A 324 | 30.812 | 65.314 | 59.096 | 1.00 56.90 | 8 |
| ATOM | 2581 | | ASN A 324 | 32.755 | 65.789 | 60.119 | 1.00 54.93 | 7 |
| ATOM | 2582 | C | ASN A 324 | 32.906 | 61.891 | 57.367 | 1.00 49.34 | 6 |
| ATOM | 2583 | ō | ASN A 324 | 32.275 | 61.502 | 56.379 | 1.00 47.22 | 8 |
| ATOM | 2584 | N | LYS A 325 | 34.182 | 61.590 | 57.586 | 1.00 48.27 | 7 |
| ATOM | 2585 | CA | LYS A 325 | 34.957 | 60.759 | 56.676 | 1.00 46.57 | 6 |
| ATOM | 2586 | CB | LYS A 325 | 36.314 | 60.453 | 57.305 | 1.00 49.94 | 6 |
| ATOM | 2587 | CG | LYS A 325 | 37.299 | 59.737 | 56.399 | 1.00 54.75 | 6 |
| ATOM | 2588 | CD | LYS A 325 | 38.562 | 59.329 | 57.173 | 1.00 58.22 | 6 |
| ATOM | 2589 | CE | LYS A 325 | 39.236 | 60.521 | 57.844 | 1.00 58.35 | 6 |
| ATOM | 2590 | NZ | LYS A 325 | 40.473 | 60.128 | 58.566 | 1.00 59.81 | 7 |
| ATOM | 2591 | С | LYS A 325 | 34.202 | 59.458 | 56.410 | 1.00 44.85 | 6 |
| ATOM | 2592 | 0 | LYS A 325 | 34.065 | 59.027 | 55.263 | 1.00 43.59 | 8 |
| ATOM | 2593 | N | ALA A 326 | 33.712 | 58.843 | 57.483 | 1.00 42.27 | 7 |
| ATOM | 2594 | CA | ALA A 326 | 32.964 | 57.597 | 57.387 | 1.00 40.91 | 6 |
| MOTA | 2595 | CB | ALA A 326 | 32.663 | 57.067 | 58.773 | 1.00 36.86 | 6 |
| MOTA | 2596 | С | ALA A 326 | 31.666 | 57.803 | 56.612 | 1.00 43.30 | 6 |
| MOTA | 2597 | 0 | ALA A 326 | 31.342 | 57.028 | 55.705 | 1.00 42.83 | 8 |
| MOTA | 2598 | N | LYS A 327 | 30.918 | 58.843 | 56.977 | 1.00 45.56 | 7 |
| MOTA | 2599 | CA | LYS A 327 | 29.657 | 59.146 | 56.306 | 1.00 47.23 | 6 6 |
| ATOM | 2600 | CB | LYS A 327 | 29.023 | 60.407 | 56.892 | 1.00 49.59 1.00 54.63 | 6 |
| MOTA | 2601 | CG | LYS A 327 | 28.547 | 60.263 61.591 | 58.329 | 1.00 55.89 | 5 |
| ATOM | 2602 | CD | LYS A 327 | 28.024 | | 58.862 60.299 | 1.00 58.28 | 6 |
| MOTA | 2603 | CE | LYS A 327 | 27.529 26.304 | 61.483 60.644 | 60.426 | 1.00 59.91 | 7 |
| ATOM | 2604 | NZ | LYS A 327 | 29.888 | 59.347 | 54.816 | 1.00 46.97 | 6 |
| ATOM | 2605 | C | LYS A 327 LYS A 327 | 29.090 | 58.913 | 53.990 | 1.00 48.10 | 8 |
| ATOM | 2606 | 0 | GLU A 328 | 30.986 | 60.012 | 54.480 | 1.00 44.99 | 7 |
| ATOM | 2607 | N | GLU A 328 | 31.325 | 60.264 | 53.091 | 1.00 43.18 | 6 |
| MOTA | 2608 2609 | CA CB | GLU A 328 | 32.417 | 61.326 | 53.027 | 1.00 47.93 | 6 |
| MOTA | 2610 | CG | GLU A 328 | 31.993 | 62.621 | 53.710 | 1.00 53.65 | 6 |
| MOTA MOTA | 2611 | CD | GLU A 328 | 33.112 | 63.630 | 53.831 | 1.00 55.79 | 6 |
| ATOM | 2612 | OE1 | GLU A 328 | 33.642 | 64.060 | 52.783 | 1.00 58.73 | 8 |
| ATOM | 2613 | OE2 | GLU A 328 | 33.459 | 63.991 | 54.979 | 1.00 58.13 | 8 |
| ATOM | 2614 | C | GLU A 328 | 31.789 | 58.971 | 52.437 | 1.00 41.56 | 6 |
| ATOM | 2615 | ō | GLU A 328 | 31.537 | 58.743 | 51.255 | 1.00 39.41 | 8 |
| ATOM | 2616 | N | LEU A 329 | 32.465 | 58.123 | 53.211 | 1.00 40.64 | 7 |
| MOTA | 2617 | CA | LEU A 329 | 32.940 | 56.844 | 52.695 | 1.00 36.45 | 6 |
| ATOM | 2618 | CB | LEU A 329 | 33.623 | 56.032 | 53.801 | 1.00 34.70 | 6 |
| ATOM | 2619 | CG | LEU A 329 | 34.100 | 54.610 | 53.433 | 1.00 35.69 | 6 |
| MOTA | 2620 | CD1 | LEU A 329 | 35.195 | 54.642 | 52.359 | 1.00 30.11 | 6 |
| ATOM | 2621 | CD2 | LEU A 329 | 34.619 | 53.926 | 54.683 | 1.00 34.63 | 6 |
| ATOM | 2622 | С | LEU A 329 | 31.746 | 56.064 | 52.157 | 1.00 35.77 | 6 |
| ATOM | 2623 | 0 | LEU A 329 | 31.692 | 55.746 | 50.975 | 1.00 34.94 | 8 |
| ATOM | 2624 | N | LEU A 330 | 30.784 | 55.770 | 53.029 | 1.00 34.78 | 7 6 |
| ATOM | 2625 | CA | LEU A 330 | 29.599 | 55.028 | 52.630 | 1.00 34.95 1.00 30.95 | 6 |
| ATOM | 2626 | CB | LEU A 330 | 28.631 | 54.914 | 53.803 | 1.00 30.95 | 6 |
| MOTA | 2627 | CG | LEU A 330 | 29.164 | 54.115 | 54.991 56.022 | 1.00 32.00 | 6 |
| MOTA | 2628 | CD1 | LEU A 330 | 28.051 | 53.904 | 54.509 | 1.00 30.73 | 6 |
| MOTA | 2629 | | LEU A 330 | 29.674 | 52.769 55.631 | 51.428 | 1.00 37.28 | 6 |
| MOTA | 2630 | C | LEU A 330 | 28.877 28.395 | 54.901 | 50.557 | 1.00 40.56 | 8 |
| ATOM | 2631 | 0 | LEU A 330 | 28.806 | 56.957 | 51.383 | 1.00 38.24 | 7 |
| MOTA | 2632 | N | LYS A 331 LYS A 331 | 28.140 | 57.661 | 50.294 | 1.00 39.59 | 6 |
| MOTA | 2633 | CA | LYS A 331 | 27.994 | 59.146 | 50.643 | 1.00 42.31 | č |
| ATOM | 2634 | CB CG | LYS A 331 | 27.129 | 59.399 | 51.873 | 1.00 45.93 | 6 |
| ATOM | 2635 | CD | LYS A 331 | 27.017 | 60.879 | 52.244 | 1.00 49.72 | 6 |
| ATOM | 2636 2637 | CE | LYS A 331 | 26.271 | 61.698 | 51.193 | 1.00 53.66 | 6 |
| ATOM | 2638 | NZ | LYS A 331 | 26.053 | 63.114 | 51.640 | 1.00 54.22 | 7 |
| ATOM | 2639 | C | LYS A 331 | 28.863 | 57.514 | 48.958 | 1.00 41.02 | 6 |
| MOTA MOTA | 2640 | Ö | LYS A 331 | 28.220 | 57.485 | 47.904 | 1.00 39.58 | 8 |
| A I UM | J-12-U | _ | | | | | | |

| | | | | | | | | | AAE | 1.00 | | 2 69 | 7. |
|-------|------|-----|---|---|-----|--------|---------|-----|--------|-------|---------|-------|-----|
| | 2641 | N | SER A 332 | | 30. | . 192 | 57.413 | | .005 | 1.00 | 44 | 2.05 | |
| ATOM | | - | | - | ì۸ | . 998 | 57.274 | 47 | .792 | 1.00 | 4 (| 6.02 | 6 |
| MOTA | 2642 | CA | SER A 332 | | | | | 4.0 | .124 | 1 00 | Δ. | 7.51 | 6 |
| | | CB | SER A 332 | | 32. | . 494 | 57.243 | | | 1.00 | | | |
| MOTA | | | | | 2 2 | .862 | 56.066 | 48 | . 823 | 1.00 |) 51 | 0.97 | 8 |
| ATOM | 2644 | OG | SER A 332 | | | | | | | 1 00 | 1 4 | 8.51 | 6 |
| | | С | SER A 332 | | 30. | . 634 | 56.007 | | .040 | 1.00 | | | |
| MOTA | 2645 | _ | 3EK 11 332 | | | .706 | 55.959 | 45 | .811 | 1.00 | 4' | 9.45 | 8 |
| ATOM | 2646 | 0 | SER A 332 - | | | | 55.555 | | | 1 00 | 5 | 1.56 | 7 |
| | _ | NT. | ILE A 333 | | 30. | .241 | 54.982 | 4. | 7.786 | 1.00 | , , | 1.50 | |
| ATOM | 2647 | N | THE R 333 | | | .869 | 53.713 | 47 | 7.187 | 1.00 |) 5 | 4.86 | 6 |
| ATOM | 2648 | CA | ILE A 333 | | | | | | | 3 00 | ٠ 5 | 5.80 | 6 |
| | | | ILE A-333 | | 29 | . 657 | 52.626 | | 3.246 | | | | |
| MOTA | 2649 | CB | | | | .388 | 51.285 | Δ- | 7.559 | 1.00 | 5 (| 2.34 | 6 |
| ATOM | 2650 | CG2 | ILE A 333 | | | | | | | | | 6.89 | 6 |
| | | CG1 | ILE A 333 | | 30 | . 892 | 52.522 | 4: | 9.140 | 1.00 | , , | 0.05 | |
| ATOM | 2651 | (61 | THE K 333 | | | .766 | 51.456 | 50 | 204 | 1.00 | ງ 6 | 0.31 | 6 |
| MOTA | 2652 | CD1 | ILE A 333 | | | | | | | 1 00 | , E | 7.07 | 6 |
| | | | ILE A 333 | | 28 | . 579 | 53.813 | | 5.396 | 1.00 | , , | 7.07 | |
| ATOM | 2653 | С | | | | .572 | 54.321 | 4 | 5.897 | 1.00 | ა 5 | 5.59 | 8 |
| MOTA | 2654 | 0 | ILE A 333 | | | | | | | 3 0/ | n 6 | 1.14 | 7 |
| | | N | ASP A 334 - | | 28 | .623 | 53.320 | | 5.160 | | | | |
| MOTA | 2655 | | 757 75 757 | | 27 | .456 | 53.300 | 4 | 4.281 | 1.00 | ე 6 | 55.55 | 6 |
| MOTA | 2656 | CA | ASP A 334 | | | | | | | 1 0 | n 6 | 9.19 | 6 |
| | 2657 | CB | ASP A 334 | | 27 | .888 | 53.259 | | 2.811 | 1.0 | J - | ,,,,, | |
| MOTA | | | | | 28 | .784 | 52.073 | 4 | 2.491 | 1.0 | 07 | 70.21 | 5 |
| ATOM | 2658 | CG | ASP A 334 | | | | | | 1.298 | 1 0 | 0.7 | 71.47 | 8 |
| | 2659 | 001 | ASP A 334 | | 29 | .097 | 51.875 | | | 1.0 | | | |
| MOTA | | | 334 | | 20 | .181 | 51.344 | 4 | 3.427 | 1.0 | 0 7 | 70.91 | 8 |
| MOTA | 2660 | OD2 | ASP A 334 | | | | | | 4.627 | 1 0 | $0 \in$ | 55.65 | 6 |
| | 2661 | С | ASP A 334 | | 26 | .660 | 52.041 | | | 1.0 | | | |
| MOTA | | | 334 | | 26 | .797 | 50.996 | 4 | 3.990 | 1.0 | 0 6 | 53.91 | 8 |
| ATOM | 2662 | 0 | ASP A 334 | • | | | | | | 1.3 | 0 6 | 65.73 | 7 |
| | 2663 | N | PHE A 335 | | 25 | .822 | 52.153 | 4 | 5.649 | 1.0 | | | |
| ATOM | | | 235 | | 25 | .041 | 51.021 | 4 | 6.104 | 1.0 | 0 6 | 63.44 | 6 |
| MOTA | 2664 | CA | PHE A 335 | | | | | | 7.632 | 1.0 | 0 5 | 58.05 | 6 |
| | 2665 | CB | PHE A 335 | | 24 | .980 | 51.034 | | | 1.0 | - : | | |
| ATOM | | | | | 24 | .039 | 50.028 | 4 | 8.195 | 1.0 | 0 : | 53.82 | 6 |
| MOTA | 2666 | CG | PHE A 335 | | | | | | 7.886 | 1.0 | 0.5 | 52.40 | 6 |
| | 2667 | CD1 | PHE A 335 | | | 1.178 | 48.679 | | | | | C1 22 | 6 |
| ATOM | | 222 | PHE A 335 | | 22 | .978 | 50.429 | 4 | 8.989 | 1.0 | ·U : | 51.33 | |
| ATOM | 2668 | CD2 | PRE A 333 | | | | 47.742 | 4 | 8.356 | 1.0 | 0 9 | 52.73 | 6 |
| ATOM | 2669 | CE1 | PHE A 335 | | | .265 | | | | 1 0 | | 53.20 | 6 |
| | | CE2 | | | 22 | 2.062 | 49.503 | 4 | 9.462 | 1.0 | /U : | 55.20 | |
| ATOM | 2670 | CEZ | PRE A 333 | | 3 | 2.204 | 48.151 | | 9.144 | 1.0 | 10 1 | 51.76 | 6 |
| ATOM | 2671 | CZ | PHE A 335 | | | | | | | 1 0 | ۱Ä. | 65.55 | 6 |
| | | C | PHE A 335 | | 23 | 3.629 | 50.893 | . 4 | 15.535 | 1.0 | ,,, | 05.55 | |
| ATOM | 2672 | C | FAL A 335 | | 2.3 | 3.230 | 49.810 | ۱ ۵ | 15.097 | 1.0 | י סנ | 67.33 | 8 |
| MOTA | 2673 | 0 | PHE A 335 | | | | | | | 1 0 | ١٥ | 66.47 | 7 |
| | | N | GLU A 336 | | 22 | 2.874 | 51.986 | , 4 | 15.537 | 1 | , , | | |
| MOTA | 2674 | | GD0 7. 330 | | 2.1 | 1.497 | 51.948 | | 15.048 | 1.0 |)0 | 67.43 | 6 |
| MOTA | 2675 | CA | GLU A 336 | | | | | | | _ | ۱0 | 71.79 | 6 |
| | 2676 | CB | GLU A 336 | | 2: | 1.422 | 51.379 | | 13.626 | | ,,, | 72.77 | |
| ATOM | | | 220 11 226 | | 3 0 | 9.982 | 51.245 | 5 4 | 13.116 | 1.0 | סכ | 78.77 | 6 |
| MOTA | 2677 | CG | GLU A 336 | | | | | | 11.789 | _ | าด | 82.67 | 6 |
| | 2678 | CD | GLU A 336 | | 1: | 9.868 | 50.505 | | | | | | 8 |
| MOTA | | | 22.17 3 22.6 | | 21 | 0.232 | 49.306 | 5 4 | 41.734 | 1.0 |)() | 83.29 | |
| ATOM | 2679 | OE1 | GLU A 336 | | | | 51.126 | | 40.801 | 1.6 | 0.0 | 84.26 | 8 |
| | 2680 | OE2 | GLU A 336 | | 1 | 9.410 | | | | | | C4 77 | 6 |
| ATOM | | | GLU A 336 | | 21 | 0.655 | 51.069 | • | 45.971 | . 1.0 | JU | 64.72 | |
| MOTA | 2681 | . C | GLU A 330 | | | | 49.840 | | 45.876 | | 00 | 59.84 | 8 |
| ATOM | 2682 | 0 | GLU A 336 | | | 0.686 | | - | | | ^^ | 64.47 | 7 |
| | | | GLU A 337 | | 1 | 9.901 | 51.710 |) | 46.858 | | | | |
| MOTA | 2683 | N | GPO Y 22, | | | | _ | | 47.805 | 1.0 | ٥٥ | 65.83 | 6 |
| MOTA | 2684 | CA | GLU A 337 | | | 9.045 | | - | | | ΛΛ. | 64.20 | 6 |
| | | CB | GLU A 337 | | 1 | 8.398 | 52.003 | | 48.759 | | 30 | 04.20 | |
| MOTA | 2685 | | GLU A 337 | | | 7.753 | | | 49.964 | 1.4 | 00 | 64.26 | 6 |
| MOTA | 2686 | CG | GLU A 337 | | | | | ~ | 50 OE | | | 64.04 | 6 |
| | _ | CD | GLU A 337 | | 1 | 8.774 | 50.6)(| U | 50.850 | | | 04.05 | - |
| MOTA | 2687 | | GEO 2: 337 | | | 9.741 | 51.3. | | 51.261 | 1. | 00 | 61.66 | 8 |
| MOTA | 2688 | OE1 | GLU A 337 | | | | | | | | ሰበ | 63.64 | 8 |
| | 2689 | OF? | 2 GLU A 337 | | 1 | 8.608 | 49.48 | | 51.132 | | | 65.00 | |
| MOTA | | | 337 | | | 7.950 | | 9 | 47.063 | 3 1. | 00 | 67.13 | 6 |
| ATOM | 2690 | С | GLU A 337 | | | | | | 46.20 | | იი | 68.27 | 8 |
| | 2691 | 0 | GLU A 337 | | 1 | 7.269 | 50.80 | , | | | | 68 33 | 7 |
| ATOM | | | 320 11 330 | | | 7.779 | | | 47.394 | 1 1. | 00 | 67.22 | |
| ATOM | 2692 | N | PHE A 338 | | | | | | 46.74 | 2 1 | വ | 68.05 | 6 |
| | 2693 | CA | PHE A 338 | | 1 | 6.764 | 48.12 | 7 | | | | 60.60 | _ |
| MOTA | | | | | | 6.445 | | 9 | 47.62 | 51. | 00 | 69.68 | 6 |
| ATOM | 2694 | CB | PHE A 338 | | | | | | 47.18 | | ሰበ | 72.35 | 6 |
| | 2695 | CG | PHE A 338 | | 1 | 5.228 | 46.15 | đ | | | | | č |
| MOTA | | | | | | 5.122 | | 4 | 45.88 | в 1. | | 72.37 | 6 |
| ATOM | 2696 | CD: | 1 PHE A 338 | | | | 45 04 | 1 | 48.07 | | 00 | 73.61 | 6' |
| | 2697 | CD. | 2 PHE A 338 | | 1 | 4.172 | | | | _ | ~~ | 72 20 | |
| MOTA | | | | | | 3.980 | | | 45.47 | 81. | 00 | 73.39 | 6 |
| ATOM | 2698 | CE: | 1 PHE A 338 | | | | | | 47.67 | | 00 | 73.26 | 6 |
| | | CE | | | 1 | 13.024 | 45.25 | U | | | | 77 74 | ē |
| ATOM | 2699 | | 7 | | | 2.929 | | 1 | 46.36 | 91. | , 00 | 73.34 | 6 |
| ATOM | 2700 | CZ | PHE A 338 | | | | | | 46.43 | | 00 | 68.45 | 6 |
| | | | PHE A 338 | | 1 | 15.48 | L 48.90 | | 40.43 | | | 67 00 | |
| ATOM | 2701 | | | | - | 5.286 | 49.36 | 57 | 45.31 | 0 1. | . 00 | 67.92 | |
| ATOM | 2702 | 0 | PHE A 338 | | | | | | 47.42 | | .00 | 68.98 | 7 |
| | | | ASP A 339 | | 1 | 14.60 | 49.02 | | | | ~~ | 70 50 | |
| atom | | | 300 3 370 | | 1 | 13.35 | | | 47.26 | 1 1. | . ບບ | 70.68 | |
| ATOM | 2704 | CA | ASP A 339 | | _ | | - 40 75 | | 48.58 | | . 00 | 71.06 | 6 |
| | | | ASP A 339 | | : | 12.59 | | | | _ | 00 | 72 05 | |
| ATOM | | | | | | 11.38 | | 78 | 48.58 | 1 1 | . UU | 72.05 | , 0 |
| 3 mOM | 2706 | CG | ASP A 339 | | | | , | - | • | | | | |

| | | | | | | | | _ |
|-------|------|---------------|---|--------|-----------------|---|------------|----|
| | 2707 | OD1 ASP A 339 | | 11.548 | 51.893 | 48.320 | 1.00 72.29 | 8 |
| ATOM | | OD2 ASP A 339 | | 10.262 | 50.188 | 48.858 | 1.00 71.03 | 8 |
| MOTA | 2708 | | | | 51.183 | 46.853 | 1.00 73.18 | 6 |
| ATOM | 2709 | C ASP A 339 | | 13.715 | | | 1.00 73.78 | 8 |
| ATOM | 2710 | O ASP A 339 | | 14.407 | 51.884 | 47.592 | 1.00 75.70 | 7 |
| | | N ASP A 340 | | 13.247 | 51.600 | 45.677 | 1.00 76.36 | |
| MOTA | 2711 | | | 13.518 | 52.943 | 45.152 | 1.00 78.34 | 6 |
| ATOM | 2712 | CA ASP A 340 | | | 53.385 | 44.189 | 1.00 77.55 | 6 |
| ATOM | 2713 | CB ASP A 340 | | 12.410 | 33.363 | | 1.00 78.90 | 6 |
| ATOM | 2714 | CG ASP A 340 | | 12.462 | 52.655 | 42.864 | | |
| | | OD1 ASP A 340 | | 12.348 | 51.408 | 42.855 | 1.00 78.38 | 8 |
| MOTA | 2715 | ODI ASI A SAO | | 12.620 | 53.336 | 41.830 | 1.00 78.74 | 8 |
| MOTA | 2716 | OD2 ASP A 340 | | | 54.017 | 46.214 | 1.00 79.51 | 6 |
| MOTA | 2717 | C ASP A 340 | - | 13.687 | | | 1.00 80.19 | 8 |
| ATOM | 2718 | O ASP A 340 | | 14.587 | 54.856 | 46.117 | | 7 |
| | | N GLU A 341 | | 12.824 | 54.000 | 47.224 | 1.00 79.64 | |
| MOTA | 2719 | | | 12.922 | 54.998 | 48.271 | 1.00 80.05 | 6 |
| ATOM | 2720 | CA GLU A 341 | | | 56.301 | 47.811 | 1.00 83.75 | 6 |
| MOTA | 2721 | CB GLU A 341 | | 12.269 | | | 1.00 89.02 | 6 |
| ATOM | 2722 | CG GLU A 341 | | 12.411 | 57.442 | 48.806 | | |
| | | CD GLU A 341 | | 11.756 | 58.724 | 48.328 | 1.00 91.52 | 6 |
| ATOM | 2723 | | | 10.515 | 58.738 | 48.175 | 1.00 93.33 | 8 |
| MOTA | 2724 | OE1 GLU A 341 | | | 59.716 | 48.102 | 1.00 92.65 | 8 |
| MOTA | 2725 | OE2 GLU A 341 | | 12.484 | | | 1.00 77.98 | 6 |
| | 2726 | C GLU A 341 | | 12.317 | 54.578 | 49.597 | 1.00 77.50 | 8 |
| ATOM | | O GLU A 341 | | 11.102 | 54.610 | 49.777 | 1.00 79.82 | |
| ATOM | 2727 | | | 13.179 | 54.181 | 50.523 | 1.00 74.49 | 7. |
| MOTA | 2728 | N VAL A 342 | | | 53.793 | 51.859 | 1.00 71.55 | 6 |
| ATOM | 2729 | CA VAL A 342 | | 12.745 | | | 1.00 72.40 | 6 |
| ATOM | 2730 | CB VAL A 342 | | 13.224 | 52.383 | 52.245 | 1.00 72.40 | 6 |
| | 2731 | CG1 VAL A 342 | | 12.672 | 52.004 | 53.610 | 1.00 71.16 | |
| MOTA | | | | 12.797 | 51.391 | 51.207 | 1.00 74.35 | 6 |
| MOTA | 2732 | | | 13.454 | 54.778 | 52.766 | 1.00 68.46 | 6 |
| MOTA | 2733 | C VAL A 342 | | | | 53.829 | 1.00 68.96 | 8 |
| ATOM | 2734 | O VAL A 342 | | 12.952 | 55.154 | | 1.00 61.61 | 7 |
| | 2735 | N ASP A 343 | | 14.636 | 55.184 | 52.311 | | |
| MOTA | | | | 15.486 | 56.114 | 53.029 | 1.00 54.91 | 6 |
| MOTA | 2736 | | | 14.678 | 57.303 | 53.543 | 1.00 55.06 | 6 |
| MOTA | 2737 | CB ASP A 343 | | | 58.390 | 54.114 | 1.00 54.44 | 6 |
| MOTA | 2738 | CG ASP A 343 | | 15.556 | | | 1.00 56.20 | 8 |
| | 2739 | OD1 ASP A 343 | | 15.002 | 59.3 5 1 | 54.694 | | |
| ATOM | | OD2 ASP A 343 | | 16.795 | 58.287 | 53.969 | 1.00 49.32 | 8 |
| ATOM | 2740 | | | 16.152 | 55.401 | 54.198 | 1.00 50.85 | 6 |
| MOTA | 2741 | C ASP A 343 | | | 55.209 | 55.257 | 1.00 49.32 | 8 |
| ATOM | 2742 | O ASP A 343 | | 15.557 | | 53.980 | 1.00 47.84 | 7 |
| MOTA | 2743 | N ARG A 344 | | 17.396 | 55.004 | | 1.00 45.34 | 6 |
| | 2744 | CA ARG A 344 | | 18.195 | 54.321 | 54.981 | 1.00 45.34 | |
| ATOM | | | | 18.883 | 53.099 | 54.358 | 1.00 45.00 | 6 |
| ATOM | 2745 | CB ARG A 344 | | 17.950 | 51.969 | 53.974 | 1.00 38.03 | 6 |
| MOTA | 2746 | CG ARG A 344 | | - | 51.531 | 55.188 | 1.00 35.83 | 6 |
| MOTA | 2747 | CD ARG A 344 | | 17.185 | | | 1.00 39.20 | 7 |
| ATOM | 2748 | NE ARG A 344 | | 16.278 | 50.439 | 54.885 | | 6 |
| - | | CZ ARG A 344 | | 15.350 | 49.993 | 55.724 | 1.00 39.89 | |
| ATOM | 2749 | CZ ARO 1. 211 | | 15.217 | 50.561 | 56.917 | 1.00 40.17 | 7 |
| ATOM | 2750 | NH1 ARG A 344 | | 14.566 | 48.976 | 55.375 | 1.00 40.75 | 7 |
| ATOM | 2751 | NH2 ARG A 344 | | 14.500 | | 55.515 | 1.00 44.72 | 6 |
| ATC I | 2752 | C ARG A 344 | | 19.250 | 55.278 | | | 8 |
| | 2753 | O ARG A 344 | | 20.170 | 54.869 | 56.223 | 1.00 46.97 | 7 |
| ATCM | | | | 19.113 | 56.552 | 55.157 | 1.00 45.81 | |
| ATC:! | 2754 | N SER A 345 | | 20.045 | 57.596 | 55.577 | 1.00 43.66 | 6 |
| ATOM | 2755 | CA SER A 345 | | | 58.960 | 55.115 | 1.00 43.44 | 6 |
| MOTA | 2756 | CB SER A 345 | | 19.538 | | 55.222 | 1.00 45.62 | 8 |
| ATOM | 2757 | OG SER A 345 | | 18.292 | 59.260 | 55.722 | 1.00 43.02 | 6 |
| | | C SER A 345 | | 20.258 | 57.627 | 57.089 | 1.00 42.79 | |
| ATOM | 2758 | C SER 7 345 | | 21.364 | 57.902 | 57.552 | 1.00 42.62 | 8 |
| ATOM | 2759 | O SER A 345 | | | | | 1.00 40.55 | 7 |
| ATOM | 2760 | N TYR A 346 | | 19.200 | | | 1.00 41.05 | 6 |
| MOTA | 2761 | CA TYR A 346 | | 19.280 | | 59.308 | 1.00 41.00 | 6 |
| | | | | 17.971 | 56.819 | | 1.00 41.74 | |
| ATOM | 2762 | | | 17.668 | | | 1.00 43.47 | 6 |
| ATOM | 2763 | CG TYR A 346 | | | | | 1.00 44.45 | 6 |
| ATOM | 2764 | CD1 TYR A 346 | | 18.331 | | | | 6 |
| | 2765 | CE1 TYR A 346 | | 18.044 | 52.983 | | | 6 |
| MOTA | | | | 16.710 | 54.988 | 58.682 | 1.00 42.08 | |
| ATOM | 2766 | | | 16.416 | 53.644 | | 1.00 40.59 | 6 |
| ATCM | 2767 | CE2 TYR A 346 | | | | | | 5 |
| ATCM | 2768 | CZ TYR A 346 | | 17:086 | | | | 8 |
| | 2769 | | | 16.806 | | | | 6 |
| ATCM | | 2.4.0 | | 20.466 | | | | |
| ATCM | 2770 | C TYR A 346 | | 21.101 | | | 1.00 42.65 | 8 |
| ATCM | 2771 | O TYR A 346 | | | | | | 7 |
| ATOM | 2772 | N MET A 347 | | 20.757 | 55.443 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | |

| | | | 245 | | 21.859 | ۱ د | 54.546 | 59.388 | 1.00 4 | 5.89 | 6 |
|--------|------|-----|-------------|---|--------|-----|--------|---------|--------|---------|-----|
| ATOM | - | CA | MET A 347 | | | | | 58.353 | 1.00 4 | 5.51 | 6 |
| ATOM | 2774 | CB | MET A 347 | | 21.950 | - | | 58.244 | 1.00 4 | 5 01 | 6 |
| ATOM | | CG | MET A 347 | | 20.727 | | | | 1.00 4 | 7 13 | 16 |
| | | SD | MET A 347 | | 21.062 | | | 57.066 | 1.00 4 | 11.22 | 6 |
| ATOM | | CE | MET A 347 | | 21.545 | | 52.237 | 55.676 | 1.00 4 | | |
| ATOM | | | MET A 347 | | 23.188 | 3 | 55.286 | 59.404 | 1.00 4 | | 6 |
| ATOM - | | C | MET A 347 | | 24.129 | | 54.888 | 60.098 | 1.00 4 | | 8 |
| MOTA | 2779 | 0 | MEI A 347 | | 23.25 | | 56.351 | 58.610 | 1.00 4 | 19.03 | 7 |
| MOTA | 2780 | N | LEU A 348 | | 24.45 | | 57.178 | 58.499 | 1.00 4 | 18.86 | 6 |
| ATOM | 2781 | ÇA | LEU A 348 | | | | 58.082 | 57.269 | 1.00 4 | 45.51 | 6 |
| ATOM | 2782 | CB | LEU A 348 | | 24.35 | | | 55.895 | 1.00 | | 6 |
| ATOM | 2783 | CG | LEU A 348 | | 24.28 | U | 57.424 | | 1.00 | 43 62 | 6 |
| ATOM | 2784 | CD1 | LEU A 348 | | 23.90 | | 58.476 | 54.859 | 1.00 | | 6 |
| ATOM | 2785 | CD2 | LEU A 348 | • | 25.61 | | 56.757 | 55.565- | 1.00 | 42.33 | 6 |
| | 2786 | C | LEU A 348 | | 24.64 | 4 | 58.049 | 59.738 | 1.00 | 49.33 | |
| ATOM | _ | 0 | LEU A 348 | | 25.76 | 5 | 58.369 | 60.123 | 1.00 | 49.78 | 8 |
| MOTA | 2787 | | GLU A 349 | | 23.53 | 7 | 58.428 | 60.358 | 1.00 | | 7 - |
| MOTA | 2788 | N | GLU A 349 | | 23.59 | | 59.279 | 61.533 | 1.00 | 49.24 | 6 |
| MOTA | 2789 | CA | | | 22.19 | | 59.848 | 61.811 | 1.00 | 48.36 | 6 |
| MOTA | 2790 | CB | GLU A 349 | | 21.62 | | 60.584 | 60.607 | 1.00 | 45.52 | 6 |
| ATOM | 2791 | CG | GLU A 349 | | 22.59 | | 61.619 | 60.065 | 1.00 | 42.94 | 6 |
| MOTA | 2792 | CD | GLU A 349 | | | | 62.560 | 60.812 | | 40.82 | 8 |
| MOTA | 2793 | OE1 | GLU A 349 | | 22.93 | | | 58.900 | | 38.30 | 8 |
| ATOM | 2794 | OE2 | GLU A 349 | | 23.02 | | 61.483 | | | 48.32 | 6 |
| ATOM | 2795 | С | GLU A 349 | | 24.11 | | 58.531 | 62.745 | | 47.87 | 8 |
| MOTA | 2796 | 0 | GLU A 349 | | 25.22 | 6 | 58.783 | 63.219 | 1.00 | | 7 |
| | 2797 | N | THR A 350 | | 23.32 | | 57.602 | 63.248 | 1.00 | 48.97 | 6 |
| ATOM | 2798 | CA | THR A 350 | | 23.74 | 4 | 56.832 | 64.398 | | 50.70 | |
| ATOM | _ | СВ | THR A 350 | | 22.55 | | 56.596 | 65.342 | 1.00 | 51.02 | 6 |
| MOTA | 2799 | 0G1 | | | 22.07 | | 57.865 | 65.803 | | 49.11 | 8 |
| MOTA | 2800 | - | | | 22.98 | | 55.763 | 66.537 | 1.00 | 51.58 | 6 |
| MOTA | 2801 | CG2 | THR A 350 | | 24.36 | | 55.507 | 63.954 | | 49.56 | 6 |
| MOTA | 2802 | C | THR A 350 | | 23.97 | | 54.947 | 62.923 | 1.00 | 50.55 | 8 |
| MOTA | 2803 | 0 | | | 25.33 | | 55.028 | 64.725 | | 46.88 | 7 |
| ATOM | 2804 | N | LEU A 351 | | 26.01 | | 53.781 | 64.417 | 1.00 | 45.35 | 6 |
| ATOM | 2805 | CA | LEU A 351 | | | | 53.726 | 65.185 | | 47.05 | 6 |
| MOTA | 2806 | CB | LEU A 351 | | 27.34 | | 52.502 | 65.072 | | 49.54 | 6 |
| ATOM | 2807 | CG | LEU A 351 | | 28.25 | | 52.777 | 65.766 | 1 00 | 51.50 | 6 |
| ATOM | 2808 | CDI | L LEU A 351 | | 29.57 | | | 65.692 | 1 00 | 48.35 | 6 |
| ATOM | 2809 | CD2 | | | 27.60 | | 51.302 | 64.772 | 1 00 | 44.79 | 6 |
| MOTA | 2810 | C | LEU A 351 | | 25.14 | | 52.584 | | | 41.45 | 8 |
| ATOM | 2811 | 0 | LEU A 351 | | 25.13 | | 51.578 | 64.061 | 1.00 | 45.27 | 7 |
| ATOM | 2812 | N | LYS A 352 | | 24.42 | | 52.711 | 65.880 | 1.00 | 44.62 | 6 |
| ATOM | 2813 | CA | LYS A 352 | | 23.5 | 31 | 51.662 | 66.375 | | | 6 |
| | 2814 | СВ | LYS A 352 | | 23.7 | 64 | 51.464 | 67.873 | 1.00 | 42.23 | 6 |
| ATOM | 2815 | CG | LYS A 352 | | 25.1 | 97 | 51.075 | 68.187 | | 44.94 | |
| ATOM | | CD | LYS A 352 | | 25.5 | 72 | 51.262 | 69.650 | 1.00 | 46.80 | 6 |
| ATOM | 2816 | CE | LYS A 352 | | 24.7 | 65 | 50.389 | 70.581 | 1.00 | 45.79 | 6 |
| MOTA | 2817 | | | | 25.2 | 36 | 50.586 | 71.975 | 1.00 | 47.31 | 7 |
| ATOM | 2818 | NZ | LYS A 352 | | 22.0 | | 52.087 | 66.116 | 1.00 | 45.12 | 6 |
| ATOM | 2819 | C | LIS A 352 | | 21.8 | | 53.236 | 65.756 | 1.00 | 47.07 | 8 |
| ATOM | 2820 | 0 | LYS A 352 | | 21.1 | | 51.161 | 66.285 | 1.00 | 44.62 | · 7 |
| ATOM | 2821 | N | ASP A 353 | | 19.7 | | 51.474 | 66.060 | 1.00 | 46.43 | 6 |
| ATOM | 2822 | CA | | | | | 50.943 | 64.692 | | 49.38 | 6 |
| ATOM | 2823 | CB | ASP A 353 | | 19.3 | | | 64.396 | 1.00 | 51.52 | 6 |
| ATOM | 2824 | CG | ASP A 353 | | 19.8 | | 49.546 | 64.158 | | 55.36 | 8 |
| MOTA | 2825 | QD | 1 ASP A 353 | | 21.0 | | 49.396 | | | 52.35 | |
| | 2826 | OD | 2 ASP A 353 | | 19.0 | | 48.596 | 64.398 | | 45 90 | |
| ATOM | 2827 | c | ASP A 353 | | 18.8 | 41 | 50.968 | 67.165 | | 45.90 | |
| ATOM | | ō | ASP A 353 | | 19.1 | 52 | 50.001 | 67.854 | | 45.98 | |
| ATOM | 2828 | | PRO A 354 | | 17.6 | 87 | 51.629 | 67.348 | 1.00 | 45.86 | |
| ATOM | 2829 | N | | | 17.1 | | 52.775 | 66.587 | | 45.36 | |
| MOTA | 2830 | CD | 7 200 7 324 | | 16.7 | | 51.243 | | 1.00 | 45.52 | 6 |
| ATOM | 2831 | CA | | | 15.5 | | 52.245 | | 1.00 | 44.77 | 6 |
| ATOM | 2832 | CB | PRO A 354 | | 15.6 | | 52.513 | | 1.00 | 45.06 | 6 |
| ATOM | 2833 | CG | PRO A 354 | | | | | | | 44.13 | 6 |
| ATOM | 2834 | C | PRO A 354 | | 16.2 | .// | 49.804 | | | 42.90 | |
| ATOM | 2835 | О | PRO A 354 | | 16.3 | | 49.271 | | | 42.77 | |
| ATOM | 2836 | | TRP A 355 | | 15.8 | | 49.174 | | | 43.35 | , 6 |
| ATOM | 2837 | | TRP A 355 | | 15.3 | | 47.801 | | | 0 47.11 | |
| | 2838 | _ | | | 14.9 | 82 | 47.225 | 70.539 | , 1.0 | | • |
| ATOM | 2000 | | ٠. | | | | | | | | |

| | | | | | | | | | - |
|--------|------|-----|-------------|---|--------|--------|----------|------------|----|
| | 0030 | ~~ | TRP A 355 | | 16.168 | 46.752 | | 1.00 52.43 | 6 |
| atom | 2839 | CG | IRF A 355 | | 16.574 | 45.391 | 71.519 | 1.00 53.15 | 6 |
| MOTA | 2840 | CD2 | TRP A 355 | | | | 72.238 | 1.00 54.97 | 6 |
| ATOM | 2841 | CE2 | TRP A 355 | | 17.789 | 45.416 | | 1.00 53.39 | 6 |
| | - | CE3 | TRP A 355 | | 16.031 | 44.153 | 71.155 | | |
| MOTA | 2842 | | TAT 355 | | 17.125 | 47.526 | 71.916 | 1.00 54.39 | 6 |
| ATOM | 2843 | CD1 | TRP A 355 | | | 46.731 | 72.468 | 1.00 57.31 | 7 |
| ATOM · | 2844 | NE1 | TRP A 355 | | 18.103 | | | 1.00 54.97 | 6 |
| | 2845 | CZ2 | TRP A 355 | | 18.469 | 44.249 | 72.602 | 1.00 54.57 | 6 |
| MOTA | _ | | TRP A 355 | | 16.706 | 42.995 | 71.518 | 1.00 55.77 | |
| MOTA | 2846 | CZ3 | TRP A 355 | | 17.913 | 43.052 | 72.234 | 1.00 54.84 | 6 |
| MOTA | 2847 | CH2 | TRP A 355 | | | | 68.230 | 1.00 41.94 | 6 |
| ATOM | 2848 | С | TRP A 355 | | 14.177 | 47.690 | | 1.00 41.39 | 8 |
| | | ō | TRP A 355 | | 13.508 | 48.677 | 67.915 | 1.00 41.33 | |
| ATOM | 2849 | | ARG A 356 | | 13.942 | 46.471 | 67.775 | 1.00 38.60 | 7 |
| MOTA | 2850 | N | ARG A 350 | | 12.855 | 46.185 | 66.866 | 1.00 36.55 | 6∙ |
| MOTA | 2851 | ·CA | ARG A 356 | | | | 65.451 | 1.00 35.06 | 6 |
| MOTA | 2852 | CB | ARG A 356 | | 13.413 | 46.044 | | 1.00 33.00 | 6 |
| | | CG | ARG A 356 | | 14.120 | 47.308 | 64.976 | 1.00 32.47 | |
| MOTA | 2853 | | ANG A 356 | | 14.969 | 47.082 | 63.733 | 1.00 29.54 | 6 |
| ATOM | 2854 | CD | ARG A 356 | | | 48.323 | 63.296 | 1.00 28.91 | 7 |
| ATOM | 2855 | NE | ARG A 356 | | 15.600 | | | 1.00 30.60 | 6 |
| | 2856 | CZ | ARG A 356 | | 16.514 | 48.403 | 62.335 | 2 00 33 53 | 7 |
| MOTA | | | 256 | | 16.916 | 47.305 | 61.702 | 1.00 33.52 | |
| MOTA | 2857 | NH1 | ANG A 350 | | 17.020 | 49.582 | 61.996 | 1.00 30.10 | 7 |
| MOTA | 2858 | NH2 | ARG A 356 | | | 44.879 | 67.361 | 1.00 36.01 | 6 |
| ATOM | 2859 | С | ARG A 356 | | 12.270 | | | 1.00 38.38 | 8 |
| | 2860 | 0 | ARG A 356 | | 12.447 | 43.831 | 66.742 | | 7 |
| MOTA | | | GLY A 357 | | 11.587 | 44.949 | 68.499 | 1.00 36.04 | |
| ATOM | 2861 | N | GD1 A 357 | | 11.001 | 43.758 | 69.085 | 1.00 36.08 | 6 |
| ATOM | 2862 | CA | GLY A 357 | | | | 68.851 | 1.00 34.51 | 6 |
| ATOM | 2863 | С | GLY A 357 | | 9.514 | 43.596 | | 1.00 36.77 | 8 |
| | 2864 | ō | GLY A 357 | | 8.943 | 44.196 | 67.943 | 1.00 30.77 | 7 |
| MOTA | | | GLY A 358 | | 8.892 | 42.772 | 69.687 | 1.00 36.04 | |
| MOTA | 2865 | N | GL1 A 330 | | 7.466 | 42.506 | 69.593 | 1.00 32.26 | 6 |
| MOTA | 2866 | CA | GLY A 358 | | | 41.263 | 70.385 | 1.00 29.85 | 6 |
| ATOM | 2867 | С | GLY A 358 | | 7.106 | | | 1.00 28.86 | 8 |
| | 2868 | ŏ | GLY A 358 | | 7.832 | 40.839 | 71.288 | 1.00 28.80 | 7 |
| MOTA | | | GLU A 359 | | 5.975 | 40.667 | 70.055 | 1.00 30.88 | |
| MOTA | 2869 | N | GLO A 323 | | 5.550 | 39.455 | 70.743 | 1.00 32.58 | 6 |
| ATOM | 2870 | CA | GLU A 359 | | | | 70.604 | 1.00 38.60 | 6 |
| ATOM | 2871 | CB | GLU A 359 | | 4.034 | 39.289 | | 1.00 47.44 | 6 |
| | | CG | GLU A 359 | | 3.230 | 40.435 | 71.222 | 1.00 47.44 | |
| MOTA | 2872 | | GLU A 359 | | 1.957 | 40.762 | 70.445 | 1.00 50.93 | 6 |
| MOTA | 2873 | CD | | | 1.123 | 39.852 | 70.221 | 1.00 52.13 | 8 |
| MOTA | 2874 | OE1 | L GLU A 359 | | | | 70.061 | 1.00 51.03 | 8 |
| ATOM | 2875 | OE2 | 2 GLU A 359 | | 1.798 | 41.942 | | 1.00 28.29 | 6 |
| | 2876 | С | GLU A 359 | | 6.250 | 38.275 | 70.091 | 1.00 20.25 | 8 |
| MOTA | | | GLU A 359 | | 6.790 | 38.382 | 68.997 | 1.00 27.88 | |
| MOTA | 2877 | 0 | GLO A 355 | | 6.263 | 37.147 | 70.772 | 1.00 27.97 | 7 |
| MOTA | 2878 | N | VAL A 360 | | | | 70.193 | 1.00 25.86 | 6 |
| ATOM | 2879 | CA | VAL A 360 | | 6.859 | 35.957 | | 1.00 22.02 | 6 |
| | 2880 | CB | VAL A 360 | | 7.673 | 35.168 | 71.237 | 1.00 22.02 | 6 |
| MOTA | | | 260 | | 8.155 | 33.849 | 70.641 | 1.00 19.45 | |
| MOTA | 2881 | CG | 1 VAL A 300 | | 8.850 | 36.009 | 71.698 | 1.00 17.88 | 6 |
| ATOM | 2882 | CG | 2 VAL A 360 | | | _ | | 1.00 28.04 | 6 |
| ATOM | 2883 | С | VAL A 360 | | 5.703 | 35.099 | | 1.00 27.34 | 8 |
| | 2884 | | VAL A 360 | | 4.842 | | | 1.00 27.34 | 7 |
| MOTA | | _ | ARG A 361 | | 5.663 | 34.898 | 68.358 | 1.00 27.70 | |
| MOTA | 2885 | N | ARG A 301 | | 4.612 | | 67.765 | 1.00 32.85 | 6 |
| MOTA | 2886 | C | ARG A 361 | | | | | 1.00 32.30 | 6 |
| MOTA | 2887 | | ARG A 361 | | 4.693 | | | 1.00 38.81 | 6 |
| | | | | | 4.243 | 35.504 | 65.687 | | |
| MOTA | 2888 | | | | 4.546 | | 64.201 | 1.00 40.09 | 6 |
| ATOM | 2889 | CD | ARG A 301 | | | | | 1.00 38.77 | 7 |
| MOTA | 2890 | NE | ARG A 361 | | 5.974 | | | 1.00 39.21 | 6 |
| | 2891 | | ARG A 361 | | 6.514 | | | | 7 |
| MOTA | | | 1 ARG A 361 | | 5.748 | 36.027 | 61.685 | 1.00 40.79 | |
| MOTA | 2892 | | T WUG W 201 | | 7.822 | | | 1.00 42.94 | 7 |
| MOTA | 2893 | NH | 2 ARG A 361 | | | | | | 6 |
| ATOM | 2894 | | ARG A 361 | | 4.689 | | | | 8 |
| | | | ARG A 361 | | 5.768 | 32.097 | 68.471 | | 7 |
| MOTA | 2895 | | TVC 3 343 | | 3.526 | | 7 68.347 | 1.00 37.80 | ' |
| MOTA | 2896 | | LYS A 362 | | 3.436 | | | 1.00 39.91 | 6 |
| MOTA | 2897 | CA | LYS A 362 | | | | | 12 12 | 6 |
| | 2898 | | | | 1.982 | | - | 45 44 | 6 |
| ATOM | | | | | 1.014 | | 3 69.640 | | 2 |
| MOTA | 2899 | | | | 1.11 | | | 1.00 49.43 | 6 |
| ATOM | | CI | LYS A 362 | | | | | | 6 |
| | | | LYS A 362 | | 0.813 | | | 44 00 | 7 |
| MOTA | | | | | 0.96 | | | | 6 |
| MOTA | | _ | 120 3 363 | | 4.32 | | | 1.00 39.25 | |
| ATOM | 2903 | | LYS A 362 | | 4.95 | | | 1.00 35.45 | 8 |
| ATOM. | | | LYS A 362 | • | 4.33 | 20.00 | | | |

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 2960 2960 2960 2960 2960 2960 2960 2960 | CAB GO CO | ASP A | 36333333333333333333333333333333333333 | 4.145.2894518875.384.0578.6679.6679.6679.6679.6679.6679.6679.66 | 26.620 25.404 24.633 23.476 25.579 25.26.478 27.445 27.445 27.445 27.445 27.495 24.105 24.105 22.995 23.21 24.461 23.72 25.63 21.68 20.65 20.65 20.65 20.65 20.65 20.65 20.05 | 68.161 68.540 67.193 66.490 65.572 64.714 64.723 67.4725 68.298 69.288 70.179 69.588 70.179 70.217 70.649 71.770 72.617 73.783 77.702 69.588 77.702 77.703 77.703 69.588 77.703 77.703 69.588 77.703 77.703 69.588 77.703 77.703 69.588 77.703 69.588 77.703 69.588 77.703 69.588 69.58 | 1.00 38.62 1.00 31.85 1.00 32.87 1.00 27.73 1.00 29.05 1.00 26.53 1.00 35.16 1.00 35.16 1.00 37.56 1.00 40.23 1.00 40.23 1.00 51.93 1.00 52.84 1.00 39.65 1.00 39.65 1.00 39.65 1.00 39.65 1.00 44.49 1.00 44.49 1.00 55.40 1.00 37.89 | 87666688687666676 |
|--|--|---|---|--|---|--|--|--|-------------------|
| • | | | | | | | | | |

| | | | | | 00 044 | 68.325 | 1.00 37.78 | 7 |
|-------|----------|---------------|----------|--------|---------|-----------|------------|---|
| ATOM | 2971 | N ALA A 37 | 1 | 11.827 | 20.944 | | 1.00 36.39 | 6 |
| | | CA ALA A 37 | 1 | 13.264 | 20.704 | | | 6 |
| | | CB ALA A 37 | 1 | 14.007 | 22.030 | • • • - • | 1.00 37.73 | |
| MOTA | | | | 13.719 | 19.972 | | 1.00 35.42 | 6 |
| ATOM | | C ALA A 37 | <u>.</u> | 14.424 | 18.964 | 69.525 | 1.00 32.06 | 8 |
| ATOM | . | O ALA A 37 | 1 | 13.317 | 20.478 | 70.766 | 1.00 33.96 | 7 |
| ATOM | 2976 | N ALA A 37 | 2 | | | 72.024 | 1.00 32.22 | 6 |
| ATOM | | CA ALA A 37 | 2 | 13.695 | 19.848 | 72.024 | 1.00 28.27 | 6 |
| | | CB ALA A 37 | 2 | 12.946 | 20.486 | 73.165 | | 6 |
| MOTA | | C ALA A 37 | 2 | 13.372 | 18.362 | 71.953 | 1.00 31.75 | |
| MOTA | | | 2 | 14.183 | 17.517 | 72.338 | 1.00 31.56 | 8 |
| MOTA | | O ALA A 37 | 2 | 12.187 | 18.059 | 71.432 | 1.00 32.72 | 7 |
| MOTA | 2981 | N ALA A 37 | 3 - | 11.710 | 16.684 | 71.305 | 1.00 32.32 | 6 |
| ATOM | 2982 | CA ALA A 37 | 3 | | 16.689 | 71.103 | 1.00 30.18 | 6 |
| ATOM | 2983 | CB ALA A 37 | '3 | 10.206 | | 70.172 | 1.00 33.13 | 6 |
| ATOM | 2984 | C ALA A 37 | '3 | 12.385 | 15.921 | | 1.00 35.87 | 8 |
| | 2985 | OT1: ALA A 37 | '3 | | 14.926 | 70.468 | 1.00 33.07 | 8 |
| MOTA | _ | OT2 ALA A 37 | 13 | 12.218 | 16.320 | 69.003 | 1.00 34.11 | |
| MOTA | 2986 | | 1 | 22.693 | 34.497 | 53.990 | 1.00 36.45 | 6 |
| MOTA | 2987 | | 1 | 35.654 | 44.211 | 49.416 | 1.00 9.27 | 8 |
| MOTA | 2988 | OH2 WAT S | | 24.480 | 33.130 | 53.069 | 1.00 21.27 | 8 |
| MOTA | 2989 | OH2 WAT S | 2 | | 30.277 | 59.314 | 1.00 14.69 | 8 |
| ATOM | 2990 | OH2 WAT S | 3 | 22.124 | | 75.741 | 1.00 27.94 | 8 |
| MOTA | 2991 | OH2 WAT S | 4 | 13.839 | 20.611 | | 1.00 44.54 | 8 |
| | 2992 | OH2 WAT S | 5 | 34.033 | 41.903 | 46.522 | 1.00 99.39 | 8 |
| MOTA | 2993 | OH2 WAT S | 6 | 15.039 | 42.130 | 55.781 | 1.00 23.79 | |
| MOTA | | OH2 WAT S | 7 | 32.737 | 41.397 | 75.900 | 1.00 15.80 | 8 |
| ATOM | 2994 | ONZ WAI S | 8 | 11.367 | 22.606 | 58.814 | 1.00 23.37 | 8 |
| MOTA | 2995 | OH2 WAT S | | 13.909 | 18.160 | 65.105 | 1.00 29.93 | 8 |
| MOTA | 2996 | OH2 WAT S | 9 | 29.655 | 56.108 | 58.029 | 1.00 50.54 | 8 |
| ATOM | 2997 | O112 - | 10 | | 17.964 | 51.885 | 1.00 9.28 | 8 |
| ATOM | 2998 | 0110 | 11 | 45.405 | | 34.515 | 1.00 32.78 | 8 |
| ATOM | 2999 | OH2 WAT S | 12 | 21.870 | 35.873 | - | 1.00 28.85 | 8 |
| | 3000 | OH2 WAT S | 13 | 43.504 | 35.670 | 33.779 | 1.00 40.53 | 8 |
| ATOM | 3001 | | 14 | 2.054 | 37.997 | 68.430 | | 8 |
| MOTA | _ | | 15 | 49.730 | 28.024 | 55.966 | 1.00 21.42 | |
| MOTA | 3002 | | 16 | 47.503 | 32.289 | 34.336 | 1.00 26.13 | 8 |
| MOTA | 3003 | | | 6.101 | 26.102 | 64.434 | 1.00 21.69 | 8 |
| MOTA | 3004 | O | 17 | 10.761 | 46.748 | 45.836 | 1.00 15.79 | 8 |
| ATOM | 3005 | OH2 WAT S | 18 | | 16.861 | 61.441 | 1.00 16.68 | 8 |
| ATOM | 3006 | OH2 WAT S | 19 | 9.146 | | 76.599 | 1.00 37.53 | 8 |
| MOTA | 3007 | OH2 WAT S | 20 | 5.684 | 34.080 | _ | 1.00 34.17 | 8 |
| | 3008 | CH2 WAT S | 21 | 14.896 | 33.163 | 49.117 | <u>-</u> | 8 |
| MOTA | 3009 | OH2 WAT S | 22 | 43.346 | 40.839 | 36.825 | | 8 |
| MOTA | | OH2 WAT S | 23 | 0.516 | 27.705 | 69.174 | 1.00 21.02 | |
| MOTA | 3010 | OH2 WAT S | 24 | 41.270 | 25.444 | 29.717 | 1.00 29.80 | 8 |
| ATOM | 3011 | | 25 | 17.818 | 29.142 | 54.584 | 1.00 27.92 | 8 |
| MOTA | 3012 | OH2 WAT S | | 21.512 | 60.572 | 56.912 | 1.00 16.77 | 8 |
| MOTA | 3013 | OH2 WAT S | 26 | 21.211 | | 48.347 | 1.00 23.93 | 8 |
| ATOM | 3014 | OH2 WAT S | 27 | | | 56.619 | 1.00 23.73 | 8 |
| ATOM | 3015 | OH2 WAT S | 28 | 47.805 | | 58.154 | 1.00 16.79 | 8 |
| ATOM | 3016 | OH2 WAT S | 2.5 | 44.624 | | | 1.00 26.61 | 8 |
| ATOM | 3017 | OH2 WAT S | 3 c | 31.096 | | 51.311 | | 8 |
| | 3018 | OH2 WAT S | 31 | 39.837 | | 55.145 | | 8 |
| ATOM | | OH2 WAT S | 32 | 11.660 | 43.601 | 63.704 | | |
| MOTA | 3019 | ONZ WAI S | 33 | 49.899 | | 53.058 | 1.00 26.85 | 8 |
| ATOM | 3020 | OH2 WAT S | 34 | 34.624 | | | 1.00 21.18 | 8 |
| MOTA | 3021 | OH2 WAT S | | | | | 1.00 27.01 | 8 |
| ATOM | 3022 | OH2 WAT S | 35 | 26.926 | | | | 8 |
| ATOM | 3023 | OH2 WAT S | 36 | 8.893 | | | | 8 |
| MOTA | 3024 | OH2 WAT S | 37 | 23.381 | | | | 8 |
| | 3025 | OH2 WAT S | 38 | 48.484 | | | | 8 |
| MOTA | | OH2 WAT S | 39 | 43.382 | 28.410 | 74.379 | | |
| ATOM | 3026 | ONS WAT S | 10 | 42.904 | | 70.272 | 1.00 29.45 | 8 |
| MOTA | 3027 | OH2 WAT 5 | | 20.521 | 53.828 | 50.298 | 1.00 22.35 | 8 |
| ATOM | 3028 | OH2 WAT S | 41 | | | | 1.00 23.32 | |
| ATOM | 3029 | OH2 WAT S | 42 | 13.310 | | | | |
| MOTA | 3030 | OH2 WAT S | 43 | 9.78 | | | | |
| | 3031 | OH2 WAT S | 44 | 36.08 | | | | |
| ATOM | 3032 | OH2 WAT S | 45 | 14.83 | | | | |
| ATOM | | OH2 WAT S | 46 | 54.16 | 2 48.19 | 4 60.971 | | 8 |
| ATOM | 3033 | | 47 | 38.94 | 3 61.29 | 63.509 | | |
| ATOM | 3034 | | 48 | 29.98 | | 2 33.130 | | |
| ATOM | 3035 | OH2 WAT S | | 31.87 | | | | 8 |
| 3 TOM | 3036 | OH2 WAT S | 49 | J1.01 | - 50.07 | • | | |

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| ATOM 3037 OH2 WAT S 50 | | | | | | | | | _ |
|--|--------|------|-------------|------------|---------|-----------------|-----------|------------|-----|
| ATOM 3038 0H2 WAT S 51 | | | C | 5.0 | 30 863 | 14.629 | 64.307 | 1.00 24.19 | 8 |
| ATOM 3019 012 WAT S 52 | ATOM | 3037 | | | | | | 1 00 27 78 | R |
| ATOM 3040 ORZ WAT S 52 | MOT/ | 3038 | OH2 WAT S | 51 | 26.119 | | | | |
| ATOM 3040 OH2 WAT S 53 ATOM 3041 OH2 WAT S 54 ATOM 3041 OH2 WAT S 55 ATOM 3042 OH2 WAT S 55 ATOM 3042 OH2 WAT S 55 ATOM 3043 OH2 WAT S 55 ATOM 3044 OH2 WAT S 55 ATOM 3044 OH2 WAT S 55 ATOM 3045 OH2 WAT S 55 ATOM 3045 OH2 WAT S 55 ATOM 3046 OH2 WAT S 55 ATOM 3046 OH2 WAT S 58 ATOM 3046 OH2 WAT S 58 ATOM 3046 OH2 WAT S 58 ATOM 3047 OH2 WAT S 58 ATOM 3046 OH2 WAT S 61 ATOM 3048 OH2 WAT S 61 ATOM 3049 OH2 WAT S 62 ATOM 3049 OH2 WAT S 62 ATOM 3049 OH2 WAT S 62 ATOM 3050 OH2 WAT S 62 ATOM 3051 OH2 WAT S 64 ATOM 3051 OH2 WAT S 64 ATOM 3051 OH2 WAT S 65 ATOM 3051 OH2 WAT S 66 ATOM 3051 OH2 WAT S 66 ATOM 3051 OH2 WAT S 66 ATOM 3053 OH2 WAT S 66 ATOM 3053 OH2 WAT S 66 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 68 ATOM 3051 OH2 WAT S 68 ATOM 3051 OH2 WAT S 68 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 68 ATOM 3051 OH2 WAT S 68 ATOM 3051 OH2 WAT S 68 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 68 ATOM 3056 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 71 ATOM 3056 OH2 WAT S 72 ATOM 3057 OH2 WAT S 72 ATOM 3057 OH2 WAT S 72 ATOM 3057 OH2 WAT S 72 ATOM 3058 OH2 WAT S 72 ATOM 3057 OH2 WAT S 72 ATOM 3057 OH2 WAT S 72 ATOM 3058 OH2 WAT S 73 ATOM 3057 OH2 WAT S 74 ATOM 3057 OH2 WAT S 74 ATOM 3058 OH2 WAT S 74 ATOM 3057 OH2 WAT S 74 ATOM 3057 OH2 WAT S 75 ATOM 3057 OH2 WAT S 78 ATOM 3058 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3058 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3058 OH2 WAT S 78 ATOM 3058 OH2 WAT S 78 ATOM 3057 OH2 WAT S 80 ATOM 3057 OH2 WAT S 80 ATOM 3057 OH2 WAT S 80 ATOM 3057 OH2 WAT S 86 ATOM 3057 OH2 WAT S 87 ATOM 3059 OH2 WAT S 87 ATOM 3059 OH2 WAT S 87 ATOM 3059 OH2 WAT S 86 ATOM 3059 OH2 WAT S 86 ATOM 3059 OH2 WAT S 86 | | | | 52 | 48.070 | 41.589 | 44.011 | | 8 |
| ATOM 3040 OR2 WAT S 54 ATOM 3041 OR2 WAT S 55 ATOM 3042 OR2 WAT S 55 ATOM 3042 OR2 WAT S 55 ATOM 3043 OR2 WAT S 55 ATOM 3044 OR2 WAT S 55 ATOM 3044 OR2 WAT S 55 ATOM 3045 OR2 WAT S 56 ATOM 3045 OR2 WAT S 57 ATOM 3046 OR2 WAT S 57 ATOM 3046 OR2 WAT S 58 ATOM 3046 OR2 WAT S 59 ATOM 3046 OR2 WAT S 59 ATOM 3047 OR2 WAT S 60 ATOM 3048 OR2 WAT S 60 ATOM 3048 OR2 WAT S 61 ATOM 3049 OR2 WAT S 62 ATOM 3050 OR2 WAT S 63 ATOM 3050 OR2 WAT S 63 ATOM 3051 OR2 WAT S 66 ATOM 3051 OR2 WAT S 66 ATOM 3051 OR2 WAT S 66 ATOM 3052 OR2 WAT S 66 ATOM 3055 OR2 WAT S 66 ATOM 3055 OR2 WAT S 66 ATOM 3056 OR2 WAT S 67 ATOM 3056 OR2 WAT S 67 ATOM 3056 OR2 WAT S 68 ATOM 3056 OR2 WAT S 67 ATOM 3056 OR2 WAT S 71 ATOM 3056 OR2 WAT S 72 ATOM 3056 OR2 WAT S 73 ATOM 3057 OR2 WAT S 73 ATOM 3058 OR2 WAT S 73 ATOM 3056 OR2 WAT S 73 ATOM 3057 OR2 WAT S 73 ATOM 3057 OR2 WAT S 73 ATOM 3058 OR2 WAT S 73 ATOM 3056 OR2 WAT S 73 ATOM 3066 OR2 WAT S 73 ATOM 3067 OR2 WAT S 73 ATOM 3067 OR2 WAT S 73 ATOM 3068 OR2 WAT S 73 ATOM 3067 OR2 WAT S 73 ATOM 3068 OR2 WAT S 73 ATOM 3067 OR2 WAT S 74 ATOM 3067 OR2 WAT S 75 ATOM 3068 OR2 WAT S 79 ATOM 3067 OR2 WAT S 88 ATOM 3068 OR2 WAT S 88 ATOM 3069 OR2 WAT S 88 ATOM 3067 OR2 WAT S 88 ATOM 3067 OR2 WAT S 88 ATOM 3067 OR2 WAT S 88 ATOM 3068 OR2 WAT S 89 ATOM 3067 OR2 WAT S 86 ATOM 3068 OR2 WAT S 86 ATOM 3069 OR2 WAT S 86 ATOM 3069 OR2 WAT S 86 | ATOM | 3039 | | | | | 52 495 | 1 00 31.04 | 8 |
| ATOM 3042 ORL WAT S 54 49.540 35.532 71.885 1.00 20.796 8 ATOM 3042 ORL WAT S 55 6.887 23.426 64.961 1.00 51.51 8 ATOM 3044 ORL WAT S 56 25.698 39.891 37.674 1.00 51.51 8 ATOM 3044 ORL WAT S 58 44.661 34.733 46.902 1.00 46.52 8 ATOM 3046 ORL WAT S 58 44.661 34.733 46.902 1.00 46.52 8 ATOM 3046 ORL WAT S 59 21.912 21.320 79.233 1.00 26.96 8 ATOM 3048 ORL WAT S 60 27.290 21.016 77.320 1.00 26.96 8 ATOM 3048 ORL WAT S 62 30.843 18.035 41.441 1.00 42.23 8 ATOM 3050 ORL WAT S 64 47.925 33.253 61.470 1.00 34.93 8 ATOM 3051 ORL WAT S 66 27.245 56.551 44.579 1.00 35.33 8 ATOM 3053 ORL WAT S 66 27.245 56.551 44.579 1.00 35.33 8 ATOM 3053 ORL WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 ORL WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 ORL WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 ORL WAT S 66 41.599 51.018 49.348 1.00 27.31 8 ATOM 3055 ORL WAT S 68 41.599 51.018 49.348 1.00 27.31 8 ATOM 3055 ORL WAT S 70 17.499 12.826 63.854 1.00 31.30 8 ATOM 3056 ORL WAT S 70 17.499 12.826 63.854 1.00 31.30 8 ATOM 3059 ORL WAT S 71 27.152 1.189 53.999 1.00 18.768 8 ATOM 3060 ORL WAT S 71 27.152 1.189 53.999 1.00 18.768 8 ATOM 3060 ORL WAT S 71 27.152 1.189 53.188 1.00 37.63 8 ATOM 3060 ORL WAT S 71 27.152 1.189 1.286 64.577 1.00 31.30 8 ATOM 3060 ORL WAT S 74 23.765 60.846 66.579 1.00 18.768 8 ATOM 3060 ORL WAT S 78 35.355 0.004 78.68 1.00 37.63 8 ATOM 3060 ORL WAT S 78 35.355 0.004 37.53 38.999 1.00 37.63 8 ATOM 3060 ORL WAT S 78 35.355 0.004 37.53 38.999 1.00 37.63 8 ATOM 3060 ORL WAT S | MOTA | 3040 | OH2 WAT S | 53 | | | | | |
| ATOM 3042 012 WAT S 555 6.887 23.426 64.961 1.00 17.49 8 ATOM 3043 012 WAT S 556 25.698 19.891 37.674 1.00 51.51 8 ATOM 3044 012 WAT S 57 45.498 44.101 55.393 1.00 37.34 8 ATOM 3045 012 WAT S 59 44.661 34.733 46.902 1.00 44.52 8 ATOM 3046 012 WAT S 59 21.912 21.320 79.233 1.00 26.96 8 ATOM 3046 012 WAT S 61 19.809 49.810 61.716 1.00 42.23 8 ATOM 3048 012 WAT S 61 19.809 49.810 61.716 1.00 42.23 8 ATOM 3049 012 WAT S 63 19.801 38.035 41.441 1.00 42.23 8 ATOM 3050 012 WAT S 63 19.853 31.379 60.511 1.00 22.74 8 ATOM 3051 012 WAT S 64 47.925 31.253 61.470 1.00 34.93 8 ATOM 3052 012 WAT S 65 32.500 36.000 41.000 1.00 34.93 8 ATOM 3053 012 WAT S 66 27.249 55.555 44.550 10.00 44.59 8 ATOM 3055 012 WAT S 66 27.249 55.555 44.579 10.00 34.19 8 ATOM 3055 012 WAT S 66 27.245 55.551 44.579 1.00 34.19 8 ATOM 3055 012 WAT S 67 5.176 32.914 54.669 1.00 41.89 8 ATOM 3055 012 WAT S 67 5.176 32.914 54.669 1.00 27.31 8 ATOM 3055 012 WAT S 67 5.176 32.914 54.669 1.00 27.31 8 ATOM 3056 012 WAT S 70 17.499 12.826 53.854 1.00 27.31 8 ATOM 3056 012 WAT S 71 27.152 12.189 33.999 1.00 18.76 8 ATOM 3056 012 WAT S 72 25.213 54.808 67.866 1.00 24.91 8 ATOM 3056 012 WAT S 72 25.213 54.808 67.866 1.00 24.91 8 ATOM 3060 012 WAT S 73 17.671 14.515 53 18.81 1.00 37.63 8 ATOM 3061 012 WAT S 74 23.765 60.846 66.579 1.00 21.81 8 ATOM 3061 012 WAT S 75 35.535 7.040 70.698 1.00 24.94 8 ATOM 3066 012 WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3067 012 WAT S 78 10.446 61.273 48.633 1.00 24.94 8 ATOM 3067 012 WAT S 78 10.446 61.273 48.633 1.00 24.94 8 ATOM 3067 012 WAT S 78 10.446 61.273 48.633 1.00 22.28 8 ATOM 3067 012 WAT S 78 10.446 61.273 48.633 1.00 22.28 8 ATOM 3067 012 WAT S 78 10.446 61.273 48.633 1.00 22.28 8 ATOM 3067 012 WAT S 88 11.456 61 27.348 62.27 1.00 35.45 8 ATOM 3067 012 WAT S 88 41.346 41.579 1.00 31.54 8 ATOM 3067 012 WAT S 89 2.26 80 34.75 1.00 31.50 8 ATOM 3067 012 WAT S 89 2.26 80 34.55 1.00 31.00 31.55 8 ATOM 3067 012 WAT S 89 2.26 80 34.55 1.00 31.00 31.50 8 ATOM 3069 012 WAT S 89 2.26 80 34.55 1.00 31.00 31.50 8 ATOM 307 | | | | 54 | 49.540 | 35.532 | 71.585 | | |
| ATOM 3042 ORZ WAT \$ 56 | ATOM | | | | | 23 426 | 64 961 | 1.00 17.49 | 8 |
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| ATOM 3044 OH2 WAT S 57 ATOM 3045 OH2 WAT S 59 ATOM 3046 OH2 WAT S 59 ATOM 3046 OH2 WAT S 59 ATOM 3046 OH2 WAT S 60 ATOM 3046 OH2 WAT S 61 ATOM 3048 OH2 WAT S 61 ATOM 3049 OH2 WAT S 62 ATOM 3050 OH2 WAT S 62 ATOM 3050 OH2 WAT S 63 ATOM 3051 OH2 WAT S 64 ATOM 3052 OH2 WAT S 63 ATOM 3052 OH2 WAT S 65 ATOM 3054 OH2 WAT S 66 ATOM 3055 OH2 WAT S 66 ATOM 3056 OH2 WAT S 66 ATOM 3056 OH2 WAT S 67 ATOM 3057 OH2 WAT S 67 ATOM 3058 OH2 WAT S 67 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 70 ATOM 3059 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3051 OH2 WAT S 70 ATOM 3052 OH2 WAT S 70 ATOM 3054 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3051 OH2 WAT S 70 ATOM 3052 OH2 WAT S 70 ATOM 3053 OH2 WAT S 70 ATOM 3054 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 80 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 80 ATOM 3050 OH2 WAT S 80 | | | | 56 | 25.698 | 39.891 | | | |
| ATOM 3045 CH2 WAT S 59 ATOM 3046 OH2 WAT S 59 ATOM 3047 OH2 WAT S 59 ATOM 3047 OH2 WAT S 59 ATOM 3047 OH2 WAT S 60 ATOM 3049 OH2 WAT S 61 ATOM 3049 OH2 WAT S 61 ATOM 3049 OH2 WAT S 62 ATOM 3050 OH2 WAT S 62 ATOM 3051 OH2 WAT S 63 ATOM 3051 OH2 WAT S 63 ATOM 3051 OH2 WAT S 63 ATOM 3052 OH2 WAT S 64 ATOM 3053 OH2 WAT S 65 ATOM 3053 OH2 WAT S 65 ATOM 3054 OH2 WAT S 65 ATOM 3055 OH2 WAT S 66 ATOM 3055 OH2 WAT S 66 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 67 ATOM 3057 OH2 WAT S 67 ATOM 3058 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3050 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 70 ATOM 3059 OH2 WAT S 78 ATOM 3057 OH2 WAT S 78 ATOM 3058 OH2 WAT S 78 ATOM 3059 OH2 WAT S 78 ATOM 3059 OH2 WAT S 80 ATOM 3051 OH2 WAT S 80 ATOM 3059 OH2 WAT S 80 ATOM 3071 OH2 WAT S 80 ATOM 3071 OH2 WAT S 80 ATOM 3072 OH2 WAT S 80 ATOM 3073 OH2 WAT S 80 ATOM 3074 OH2 WAT S 80 ATOM 3075 OH2 WAT S 80 ATOM 3075 OH2 WAT S 80 ATOM 3070 OH2 WAT S 80 ATOM 3071 OH2 WAT S 80 ATOM 3071 OH2 WAT S 80 ATOM 3071 OH2 WAT S 80 ATOM 3074 OH2 WAT S 80 ATOM 3075 OH2 WAT S 80 | ATOM | | | | 45 498 | 44.101 | 55.393 | 1.00 37.34 | 8 |
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| ATOM 3047 OH2 WAT S 60 17.390 21.016 77.320 1.00 27.74 8 ATOM 3040 OH2 WAT S 61 19.809 49.810 61.716 1.00 46.14 8 ATOM 3040 OH2 WAT S 62 30.843 18.035 41.441 1.00 42.23 8 ATOM 3051 OH2 WAT S 63 19.055 33.379 60.511 1.00 28.99 8 ATOM 3051 OH2 WAT S 65 32.500 33.379 60.511 1.00 28.99 8 ATOM 3053 OH2 WAT S 66 27.245 56.551 44.579 1.00 34.93 8 ATOM 3053 OH2 WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3053 OH2 WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 OH2 WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 OH2 WAT S 69 12.869 50.298 61.877 1.00 31.30 8 ATOM 3056 OH2 WAT S 70 17.499 12.826 63 854 1.00 24.91 8 ATOM 3056 OH2 WAT S 70 17.499 12.826 63 854 1.00 24.91 8 ATOM 3058 OH2 WAT S 71 27.152 12.189 53.999 1.00 18.76 8 ATOM 3058 OH2 WAT S 72 25.213 54.809 67.866 1.00 61.35 8 ATOM 3050 OH2 WAT S 73 17.671 48.515 53.188 1.00 37.63 8 ATOM 3060 OH2 WAT S 73 27.761 48.515 53.188 1.00 37.63 8 ATOM 3060 OH2 WAT S 73 27.614 48.515 53.188 1.00 37.63 8 ATOM 3063 OH2 WAT S 74 22.755 60.846 66.579 1.00 21.81 8 ATOM 3065 OH2 WAT S 76 26.280 16.065 76.556 1.00 61.35 8 ATOM 3065 OH2 WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3066 OH2 WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3067 OH2 WAT S 88 12.989 118.071 46.109 1.00 22.84 8 ATOM 3069 OH2 WAT S 88 12.989 118.071 46.109 1.00 22.84 8 ATOM 3069 OH2 WAT S 88 12.866 24.723 75.807 1.00 35.31 8 ATOM 3069 OH2 WAT S 88 12.864 27.73 75.807 1.00 35.31 8 ATOM 3069 OH2 WAT S 88 12.864 27.73 75.807 1.00 35.31 8 ATOM 3069 OH2 WAT S 89 12.864 69.297 7.10 0.00 35.31 8 ATOM 3069 OH2 WAT S 89 12.866 69.297 7.10 0.00 35.31 8 ATOM 3069 OH2 WAT S 89 13.256 24.051 73.017 1.00 35.45 8 ATOM 3079 OH2 WAT S 89 18.256 24.051 73.017 1.00 35.45 8 ATOM 3079 OH2 WAT S 89 18.340 89 18.00 30.71 8 ATOM 3079 OH2 WAT S 89 18.340 89 18.00 30.71 8 ATOM 3079 OH2 WAT S 89 18.340 89 27.755 11.00 34.73 8 ATOM 3079 OH2 WAT S 89 18.340 89 27.755 11.00 34.73 8 ATOM 3080 OH2 WAT S 99 26.00 84.552 29.97 74.111 1.00 25.23 8 ATOM 3080 OH2 WAT S 99 25.00 8 8.340 77.358 1.00 44.60 99 8 ATOM 3090 OH2 WA | | | OND HAM C | 50 | 21 912 | 21.320 | 79.233 | 1.00 26.96 | 8 |
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| ATOM 3048 OH2 WAT S 61 ATOM 3049 OH2 WAT S 62 ATOM 3050 OH2 WAT S 63 ATOM 3050 OH2 WAT S 63 ATOM 3050 OH2 WAT S 63 ATOM 3050 OH2 WAT S 64 ATOM 3051 OH2 WAT S 65 ATOM 3052 OH2 WAT S 65 ATOM 3052 OH2 WAT S 65 ATOM 3053 OH2 WAT S 66 ATOM 3054 OH2 WAT S 66 ATOM 3054 OH2 WAT S 66 ATOM 3055 OH2 WAT S 66 ATOM 3056 OH2 WAT S 67 ATOM 3056 OH2 WAT S 69 ATOM 3056 OH2 WAT S 70 ATOM 3057 OH2 WAT S 70 ATOM 3058 OH2 WAT S 70 ATOM 3059 OH2 WAT S 71 ATOM 3059 OH2 WAT S 71 ATOM 3050 OH2 WAT S 72 ATOM 3050 OH2 WAT S 72 ATOM 3050 OH2 WAT S 73 ATOM 3050 OH2 WAT S 74 ATOM 3051 OH2 WAT S 74 ATOM 3051 OH2 WAT S 75 ATOM 3061 OH2 WAT S 75 ATOM 3062 OH2 WAT S 75 ATOM 3063 OH2 WAT S 76 ATOM 3064 OH2 WAT S 77 ATOM 3065 OH2 WAT S 76 ATOM 3066 OH2 WAT S 77 ATOM 3067 OH2 WAT S 79 ATOM 3068 OH2 WAT S 79 ATOM 3069 OH2 WAT S 79 ATOM 3069 OH2 WAT S 81 ATOM 3069 OH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3069 OH2 WAT S 83 ATOM 3069 OH2 WAT S 83 ATOM 3069 OH2 WAT S 86 ATOM 3069 OH2 WAT S 86 ATOM 3069 OH2 WAT S 88 ATOM 3069 OH2 WAT S 89 ATOM 3069 OH2 WAT S 88 ATOM 3069 OH2 WAT S 89 ATOM 3070 OH2 WAT S 88 ATOM 3071 OH2 WAT S 89 ATOM 3071 OH2 WAT S 89 ATOM 3071 OH2 WAT S 89 ATOM 3072 OH2 WAT S 89 ATOM 3073 OH2 WAT S 89 ATOM 3073 OH2 WAT S 89 ATOM 3074 OH2 WAT S 89 ATOM 3075 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3080 OH2 WAT S 99 | MOTA | 3047 | OH2 WAT S | 60 | | | | | |
| ATOM 3049 OH2 WAT 5 62 30.883 18.035 41.441 1.00 42.23 8 ATOM 3050 OH2 WAT 5 63 19.055 33.379 60.511 1.00 28.99 8 ATOM 3051 OH2 WAT 5 64 47.925 33.253 61.470 1.00 34.93 8 ATOM 3051 OH2 WAT 5 65 32.500 36.000 41.000 1.00 35.33 8 ATOM 3052 OH2 WAT 5 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3053 OH2 WAT 5 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3055 OH2 WAT 5 68 41.159 51.018 49.348 1.00 27.31 8 ATOM 3055 OH2 WAT 5 68 41.159 51.018 49.348 1.00 27.31 8 ATOM 3055 OH2 WAT 5 70 17.499 12.826 63.854 1.00 24.91 8 ATOM 3057 OH2 WAT 5 70 17.499 12.826 63.854 1.00 24.91 8 ATOM 3059 OH2 WAT 5 71 27.152 12.189 50.298 61.877 1.00 31.30 8 ATOM 3059 OH2 WAT 5 72 25.13 54.809 67.866 1.00 61.35 8 ATOM 3059 OH2 WAT 5 72 25.13 54.809 67.866 1.00 61.35 8 ATOM 3060 OH2 WAT 5 72 25.13 54.809 67.866 1.00 61.35 8 ATOM 3060 OH2 WAT 5 75 35.555 27.040 70.698 1.00 34.04 8 ATOM 3061 OH2 WAT 5 75 35.555 27.040 70.698 1.00 34.04 8 ATOM 3063 CH2 WAT 5 77 18.451 25.555 45.150 1.00 28.55 8 ATOM 3063 OH2 WAT 5 77 18.451 25.555 45.150 1.00 22.20 8 ATOM 3066 OH2 WAT 5 77 18.451 25.555 45.150 1.00 28.55 8 ATOM 3066 OH2 WAT 5 78 10.466 61.273 48.633 1.00 44.74 8 ATOM 3066 OH2 WAT 5 78 10.466 61.273 48.633 1.00 44.74 8 ATOM 3067 OH2 WAT 5 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 OH2 WAT 5 88 12.886 42.723 75.807 1.00 35.45 8 ATOM 3067 OH2 WAT 5 88 12.886 42.723 75.807 1.00 35.45 8 ATOM 3070 OH2 WAT 5 88 13.406 44.647 71.349 1.00 35.45 8 ATOM 3070 OH2 WAT 5 88 13.406 44.647 71.349 1.00 47.24 8 ATOM 3070 OH2 WAT 5 88 13.406 44.647 71.349 1.00 47.24 8 ATOM 3070 OH2 WAT 5 88 13.406 44.647 71.349 1.00 49.99 8 ATOM 3070 OH2 WAT 5 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3070 OH2 WAT 5 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3070 OH2 WAT 5 89 50.621 36.644 60.244 1.00 19.51 8 ATOM 3070 OH2 WAT 5 89 50.621 36.644 60.244 1.00 19.51 8 ATOM 3070 OH2 WAT 5 89 50.661 38.453 1.00 44.74 8 89 50.621 36.644 60.244 1.00 37.74 8 8 340 340 340 340 340 340 340 340 340 340 | | | OUR WAT S | 61 | 19.809 | 49.810 | | | |
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| ATOM 3050 OHZ WAT S 64 47.925 33.3.39 61.470 1.00 34.93 8 ATOM 3051 OHZ WAT S 65 47.925 33.3.253 61.470 1.00 34.93 8 ATOM 3052 OHZ WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3053 OHZ WAT S 66 27.245 56.551 44.579 1.00 34.19 8 ATOM 3054 OHZ WAT S 68 41.159 51.018 49.348 1.00 27.31 8 ATOM 3055 OHZ WAT S 68 41.159 51.018 49.348 1.00 27.31 8 ATOM 3056 OHZ WAT S 69 12.869 50.298 61.877 1.00 31.30 8 ATOM 3057 OHZ WAT S 71 27.152 12.189 53.999 1.00 18.76 8 ATOM 3059 OHZ WAT S 72 25.213 54.809 67.866 1.00 61.35 8 ATOM 3060 OHZ WAT S 73 17.671 48.515 53.188 1.00 37.63 8 ATOM 3061 OHZ WAT S 75 35.535 27.040 70.698 1.00 34.04 8 ATOM 3064 OHZ WAT S 75 35.535 27.040 70.698 1.00 34.04 8 ATOM 3065 OHZ WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3066 OHZ WAT S 79 13.256 24.617 30.17 1.00 31.30 8 ATOM 3066 OHZ WAT S 79 13.256 24.617 30.07 1.00 37.63 8 ATOM 3066 OHZ WAT S 79 13.256 24.617 30.07 1.00 37.63 8 ATOM 3066 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3067 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3067 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3076 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3076 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3076 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3076 OHZ WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3076 OHZ WAT S 80 23.571 13.292 69.937 1.00 49 | ATOM | 3049 | OH2 WAT S | | | | | | Q |
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| ATOM 3055 OH2 WAT \$ 68 | ATOM | | UNZ WAT S | | | 32 914 | 54.669 | 1.00 41.89 | 8 |
| ATOM 3055 OH2 WAT \$ 68 | ATOM | 3054 | OH2 WAT 5 | | | | | | a |
| ATOM 3056 CH2 WAT S 70 17.499 12.826 63.854 1.00 24.91 8 ATOM 3058 OH2 WAT S 71 27.152 12.189 53.999 1.00 18.76 8 ATOM 3059 OH2 WAT S 72 25.213 54.809 67.866 1.00 31.35 8 ATOM 3060 OH2 WAT S 73 17.671 48.515 53.188 1.00 37.63 8 ATOM 3061 OH2 WAT S 75 35.555 27.040 70.698 1.00 31.03 8 ATOM 3062 CH2 WAT S 75 35.555 27.040 70.698 1.00 31.03 4.04 8 ATOM 3063 CH2 WAT S 76 26.280 16.065 76.564 1.00 32.20 8 ATOM 3064 CH2 WAT S 77 18.451 25.555 45.150 1.00 28.55 8 ATOM 3066 CH2 WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3066 CH2 WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 CH2 WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 CH2 WAT S 81 29.881 18.071 46.109 1.00 22.84 8 ATOM 3069 CH2 WAT S 83 41.348 15.471 45.004 1.00 49.67 8 ATOM 3070 CH2 WAT S 83 41.348 15.471 45.004 1.00 49.67 8 ATOM 3071 CH2 WAT S 85 5.217 40.817 61.244 1.00 19.51 8 ATOM 3072 CH2 WAT S 87 8.881 21.532 56.838 1.00 30.72 8 ATOM 3073 CH2 WAT S 88 41.816 25.022 72.452 1.00 30.72 8 ATOM 3076 CH2 WAT S 89 50.621 36.644 66.93 1.00 31.50 8 ATOM 3077 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3079 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3079 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 89 50.621 36.644 6.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 91 8.131 39.168 54.093 1.00 31.50 8 ATOM 3080 CH2 WAT S 92 16.591 58.091 57.551 1.00 33.77 8 ATOM 3080 CH2 WAT S 92 16.591 58.091 57.551 1.00 33.77 8 ATOM 3080 CH2 WAT S 94 42.105 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 92 16.591 58.091 57.551 1.00 33.77 8 ATOM 3080 CH2 WAT S 99 22.608 32.989 62.927 1.00 50.77 8 ATOM 3080 CH2 WAT S 99 22.608 34.532 49.627 1.00 46.63 8 ATOM 3080 CH2 WAT S 99 22.608 59.572 1.00 35.49 8 ATOM 3080 CH2 WAT S 100 44.77 47.426 38.893 1.00 31.60 8 ATOM 3080 CH2 WAT S 100 44.247 7 1.77 46.986 1.00 44.26 8 ATOM 3080 CH2 WAT S 100 44.247 7 1.77 46.986 1.00 44.26 8 ATOM | | 3055 | OH2 WAT S | 68 | 41.159 | 21.018 | | | |
| ATOM 3057 OH2 WAT \$ 70 ATOM 3058 OH2 WAT \$ 71 ATOM 3058 OH2 WAT \$ 71 ATOM 3058 OH2 WAT \$ 72 ATOM 3059 OH2 WAT \$ 72 ATOM 3060 OH2 WAT \$ 72 ATOM 3060 OH2 WAT \$ 74 ATOM 3061 OH2 WAT \$ 74 ATOM 3062 CH2 WAT \$ 75 ATOM 3062 CH2 WAT \$ 75 ATOM 3063 CH2 WAT \$ 75 ATOM 3064 OH2 WAT \$ 76 ATOM 3064 OH2 WAT \$ 76 ATOM 3065 CH2 WAT \$ 77 ATOM 3066 CH2 WAT \$ 77 ATOM 3066 CH2 WAT \$ 77 ATOM 3066 CH2 WAT \$ 78 ATOM 3066 OH2 WAT \$ 78 ATOM 3066 CH2 WAT \$ 78 ATOM 3066 CH2 WAT \$ 79 ATOM 3066 CH2 WAT \$ 80 ATOM 3066 CH2 WAT \$ 80 ATOM 3067 OH2 WAT \$ 80 ATOM 3068 CH2 WAT \$ 81 ATOM 3069 OH2 WAT \$ 82 ATOM 3070 OH2 WAT \$ 82 ATOM 3070 OH2 WAT \$ 82 ATOM 3071 CH2 WAT \$ 85 ATOM 3071 CH2 WAT \$ 85 ATOM 3072 CH2 WAT \$ 85 ATOM 3073 OH2 WAT \$ 85 ATOM 3074 CH2 WAT \$ 88 ATOM 3075 CH2 WAT \$ 88 ATOM 3076 CH2 WAT \$ 88 ATOM 3076 CH2 WAT \$ 88 ATOM 3077 CH2 WAT \$ 88 ATOM 3070 CH2 WAT \$ 87 ATOM 3071 CH2 WAT \$ 87 ATOM 3071 CH2 WAT \$ 87 ATOM 3072 CH2 WAT \$ 87 ATOM 3073 CH2 WAT \$ 89 ATOM 3074 CH2 WAT \$ 89 ATOM 3075 CH2 WAT \$ 89 ATOM 3076 CH2 WAT \$ 89 ATOM 3076 CH2 WAT \$ 89 ATOM 3077 CH2 WAT \$ 89 ATOM 3078 CH2 WAT \$ 99 ATOM 3079 CH2 WAT \$ 99 ATOM 3070 CH2 WAT \$ 99 ATOM 3080 CH2 WAT \$ 100 ATOM 3080 | | | OTTO WATE | 69 | 12.869 | 50.298 | 61.877 | 1.00 31.30 | 8 |
| ATOM 3058 OH2 WAT S 71 | MOTA | | OHZ WAI 5 | | | | 63 R54 | 1.00 24.91 | 8 |
| ATOM 3058 OH2 WAT S 72 ATOM 3060 OH2 WAT S 72 ATOM 3061 OH2 WAT S 73 ATOM 3061 OH2 WAT S 74 ATOM 3061 OH2 WAT S 75 ATOM 3062 CH2 WAT S 75 ATOM 3064 OH2 WAT S 75 ATOM 3065 CH2 WAT S 75 ATOM 3066 OH2 WAT S 77 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 80 ATOM 3066 OH2 WAT S 80 ATOM 3067 OH2 WAT S 80 ATOM 3069 OH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 82 ATOM 3070 OH2 WAT S 83 ATOM 3070 OH2 WAT S 84 ATOM 3071 OH2 WAT S 85 ATOM 3070 OH2 WAT S 86 ATOM 3070 OH2 WAT S 87 ATOM 3070 OH2 WAT S 88 ATOM 3070 OH2 WAT S 87 ATOM 3070 OH2 WAT S 88 ATOM 3070 OH2 WAT S 87 ATOM 3070 OH2 WAT S 87 ATOM 3070 OH2 WAT S 88 ATOM 3070 OH2 WAT S 87 ATOM 3070 OH2 WAT S 89 ATOM 3070 OH2 WAT S 90 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 100 ATOM 3080 O | MOTA | 3057 | | | | | | | |
| ATOM 3059 OH2 WAT S 72 ATOM 3060 OH2 WAT S 73 ATOM 3060 OH2 WAT S 74 ATOM 3061 OH2 WAT S 74 ATOM 3061 OH2 WAT S 74 ATOM 3062 CH2 WAT S 75 ATOM 3063 CH2 WAT S 76 ATOM 3064 OH2 WAT S 76 ATOM 3065 CH2 WAT S 76 ATOM 3066 OH2 WAT S 77 ATOM 3066 OH2 WAT S 77 ATOM 3066 OH2 WAT S 77 ATOM 3066 OH2 WAT S 79 ATOM 3067 OH2 WAT S 79 ATOM 3067 OH2 WAT S 80 ATOM 3067 OH2 WAT S 81 ATOM 3069 OH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 84 ATOM 3073 OH2 WAT S 85 ATOM 3073 OH2 WAT S 86 ATOM 3075 OH2 WAT S 86 ATOM 3075 OH2 WAT S 87 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 87 ATOM 3078 OH2 WAT S 87 ATOM 3079 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3080 OH2 WAT S 89 ATOM 3080 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3080 OH2 WAT S 89 ATOM 3099 OH2 WAT S 89 ATOM 3088 OH2 WAT S 99 ATOM 3089 OH2 WAT S 99 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 WAT S 100 A | | | OHO WAT S | 71 | 27.152 | 12.189 | | | |
| ATOM 3060 OHZ WAT S 73 ATOM 3061 OHZ WAT S 74 ATOM 3061 OHZ WAT S 74 ATOM 3061 OHZ WAT S 75 ATOM 3063 CHZ WAT S 75 ATOM 3063 CHZ WAT S 75 ATOM 3064 OHZ WAT S 76 ATOM 3065 CHZ WAT S 77 ATOM 3066 OHZ WAT S 77 ATOM 3066 OHZ WAT S 78 ATOM 3067 OHZ WAT S 80 ATOM 3067 OHZ WAT S 81 ATOM 3068 CHZ WAT S 81 ATOM 3069 OHZ WAT S 82 ATOM 3070 OHZ WAT S 82 ATOM 3071 OHZ WAT S 83 ATOM 3070 OHZ WAT S 84 ATOM 3071 OHZ WAT S 85 ATOM 3071 OHZ WAT S 85 ATOM 3072 OHZ WAT S 85 ATOM 3073 OHZ WAT S 85 ATOM 3074 CHZ WAT S 87 ATOM 3075 OHZ WAT S 88 ATOM 3075 OHZ WAT S 88 ATOM 3076 OHZ WAT S 88 ATOM 3077 OHZ WAT S 88 ATOM 3077 OHZ WAT S 88 ATOM 3078 OHZ WAT S 89 ATOM 3079 OHZ WAT S 89 ATOM 3070 OHZ WAT S 89 ATOM 3070 OHZ WAT S 89 ATOM 3070 OHZ WAT S 88 ATOM 3070 OHZ WAT S 88 ATOM 3070 OHZ WAT S 87 ATOM 3075 OHZ WAT S 87 ATOM 3076 OHZ WAT S 88 ATOM 3077 OHZ WAT S 88 ATOM 3077 OHZ WAT S 88 ATOM 3078 OHZ WAT S 89 ATOM 3080 OHZ WAT S 89 ATOM 3080 OHZ WAT S 90 ATOM 3080 OHZ WAT S 90 ATOM 3080 OHZ WAT S 93 ATOM 3080 OHZ WAT S 93 ATOM 3081 OHZ WAT S 94 ATOM 3082 OHZ WAT S 94 ATOM 3083 OHZ WAT S 93 ATOM 3084 OHZ WAT S 99 ATOM 3085 OHZ WAT S 99 ATOM 3086 OHZ WAT S 99 ATOM 3087 OHZ WAT S 99 ATOM 3088 OHZ WAT S 99 ATOM 3089 OHZ WAT S 99 ATOM 3080 OHZ WAT S 101 ATOM 3080 OHZ WAT S 102 ATOM 3080 OHZ WAT S 103 ATOM 3080 OHZ WAT S 104 ATOM 3080 OHZ WAT S 106 A | | | 0112 WATE C | | 25 213 | 54.809 | 67.866 | 1.00 61.35 | 8 |
| ATOM 3060 OH2 WAT S 74 ATOM 3061 OH2 WAT S 74 ATOM 3062 CH2 WAT S 75 ATOM 3063 CH2 WAT S 76 ATOM 3063 CH2 WAT S 76 ATOM 3064 OH2 WAT S 77 ATOM 3065 CH2 WAT S 77 ATOM 3065 CH2 WAT S 77 ATOM 3066 CH2 WAT S 78 ATOM 3066 CH2 WAT S 79 ATOM 3066 CH2 WAT S 80 ATOM 3066 CH2 WAT S 81 ATOM 3066 CH2 WAT S 82 ATOM 3067 OH2 WAT S 82 ATOM 3069 CH2 WAT S 82 ATOM 3070 CH2 WAT S 84 ATOM 3070 CH2 WAT S 84 ATOM 3071 CH2 WAT S 85 ATOM 3072 CH2 WAT S 85 ATOM 3073 CH2 WAT S 85 ATOM 3074 CH2 WAT S 86 ATOM 3075 CH2 WAT S 88 ATOM 3075 CH2 WAT S 87 ATOM 3076 CH2 WAT S 89 ATOM 3077 CH2 WAT S 89 ATOM 3077 CH2 WAT S 89 ATOM 3078 CH2 WAT S 89 ATOM 3079 CH2 WAT S 89 ATOM 3079 CH2 WAT S 89 ATOM 3080 CH2 WAT S 90 ATOM 3080 CH2 WAT S 100 ATOM 3090 CH2 WAT S | ATOM | 3059 | OHZ WAT S | | | | | 1 00 37 63 | 8 |
| ATOM 3061 OH2 WAT S 75 ATOM 3062 CH2 WAT S 75 ATOM 3063 CH2 WAT S 76 ATOM 3064 OH2 WAT S 77 ATOM 3065 OH2 WAT S 77 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 78 ATOM 3066 OH2 WAT S 80 ATOM 3066 OH2 WAT S 80 ATOM 3067 OH2 WAT S 81 ATOM 3068 OH2 WAT S 81 ATOM 3069 OH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 83 ATOM 3071 CH2 WAT S 84 ATOM 3071 CH2 WAT S 84 ATOM 3073 OH2 WAT S 85 ATOM 3073 OH2 WAT S 86 ATOM 3073 OH2 WAT S 86 ATOM 3074 CH2 WAT S 88 ATOM 3075 OH2 WAT S 88 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3078 OH2 WAT S 89 ATOM 3079 OH2 WAT S 90 ATOM 3080 OH2 WAT S 91 ATOM 3080 OH2 WAT S 91 ATOM 3080 OH2 WAT S 92 ATOM 3080 OH2 WAT S 94 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 WAT | ATOM | 3060 | OH2 WAT S | 73 | | | | | |
| ATOM 3062 CH2 WAT S 75 35.535 27.040 76.598 1.00 32.20 8 ATOM 3063 CH2 WAT S 76 26.280 16.065 76.564 1.00 32.20 8 ATOM 3064 CH2 WAT S 77 18.451 25.555 45.150 1.00 28.55 8 ATOM 3065 CH2 WAT S 78 10.446 61.273 48.633 1.00 44.74 8 ATOM 3066 CH2 WAT S 80 23.571 13.292 69.937 1.00 49.49 8 ATOM 3066 CH2 WAT S 81 29.891 18.071 46.109 1.00 22.84 8 ATOM 3068 CH2 WAT S 82 21.886 42.773 75.807 1.00 35.31 8 ATOM 3069 CH2 WAT S 83 41.3406 44.647 71.349 1.00 47.24 8 ATOM 3071 CH2 WAT S 84 13.406 44.647 71.349 1.00 47.24 8 ATOM 3073 CH2 WAT S 85 30.444 35.217 51.882 1.00 38.15 8 ATOM 3073 CH2 WAT S 85 30.444 35.217 51.882 1.00 38.15 8 ATOM 3076 CH2 WAT S 88 8.891 21.532 56.838 1.00 30.72 8 ATOM 3076 CH2 WAT S 89 50.621 36.644 60.248 1.00 22.92 8 ATOM 3076 CH2 WAT S 89 50.621 36.644 60.248 1.00 22.92 8 ATOM 3078 CH2 WAT S 90 81.31 39.168 54.903 1.00 31.50 8 ATOM 3079 CH2 WAT S 91 81.31 39.168 54.903 1.00 31.50 8 ATOM 3080 CH2 WAT S 93 34.773 54.055 69.382 1.00 36.05 8 ATOM 3080 CH2 WAT S 94 42.105 31.720 71.257 1.00 35.47 8 ATOM 3083 CH2 WAT S 99 42.105 31.720 71.257 1.00 35.49 8 ATOM 3086 CH2 WAT S 99 42.105 31.720 71.257 1.00 35.49 8 ATOM 3086 CH2 WAT S 99 42.105 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 99 42.105 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 99 42.105 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 99 42.106 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 99 42.106 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 99 42.106 31.720 71.257 1.00 35.49 8 ATOM 3080 CH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3080 CH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3090 CH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3090 CH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3090 CH2 WAT S 100 37.304 39.027 73.722 1.00 35.49 8 ATOM 3090 CH2 WAT S 103 40.24 42.997 74.111 1.00 25.23 8 ATOM 3090 CH2 WAT S 100 40.850 36.936 31.885 1.00 40.03 8 ATOM 3090 CH2 WAT S 100 40.850 36.936 31.885 1.00 40.03 8 ATOM 3090 CH2 WAT S 100 40.95 8 ATOM 3090 CH2 WAT S 100 40.95 8 ATOM 3090 CH2 WAT S 100 40.95 8 ATOM 30 | | | OHO WAT S | 74 | 23.765 | 60.846 | | | |
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| ATOM 3064 OH2 WAT S 78 ATOM 3065 CH2 WAT S 78 ATOM 3066 OH2 WAT S 79 ATOM 3066 OH2 WAT S 79 ATOM 3066 OH2 WAT S 79 ATOM 3066 OH2 WAT S 80 ATOM 3068 CH2 WAT S 80 ATOM 3068 OH2 WAT S 80 ATOM 3069 OH2 WAT S 80 ATOM 3070 OH2 WAT S 82 ATOM 3070 OH2 WAT S 83 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 84 ATOM 3072 OH2 WAT S 85 ATOM 3073 OH2 WAT S 85 ATOM 3074 OH2 WAT S 85 ATOM 3075 OH2 WAT S 86 ATOM 3076 OH2 WAT S 87 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3078 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3079 OH2 WAT S 89 ATOM 3070 OH2 WAT S 89 ATOM 3077 OH2 WAT S 90 ATOM 3078 OH2 WAT S 91 ATOM 3078 OH2 WAT S 91 ATOM 3080 OH2 WAT S 92 ATOM 3080 OH2 WAT S 93 ATOM 3081 OH2 WAT S 93 ATOM 3081 OH2 WAT S 95 ATOM 3083 OH2 WAT S 96 ATOM 3083 OH2 WAT S 96 ATOM 3084 OH2 WAT S 96 ATOM 3085 OH2 WAT S 98 ATOM 3086 OH2 WAT S 99 ATOM 3087 OH2 WAT S 99 ATOM 3088 OH2 WAT S 99 ATOM 3088 OH2 WAT S 99 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 WAT | ATOM | 3063 | | | | | | | |
| ATOM 3066 CH2 WAT S 78 ATOM 3066 CH2 WAT S 79 ATOM 3066 CH2 WAT S 80 ATOM 3067 OH2 WAT S 80 ATOM 3068 CH2 WAT S 81 ATOM 3068 CH2 WAT S 81 ATOM 3068 CH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 82 ATOM 3070 CH2 WAT S 83 ATOM 3071 CH2 WAT S 84 ATOM 3071 CH2 WAT S 84 ATOM 3072 CH2 WAT S 85 ATOM 3073 OH2 WAT S 85 ATOM 3074 CH2 WAT S 86 ATOM 3075 CH2 WAT S 87 ATOM 3076 CH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 89 ATOM 3078 CH2 WAT S 89 ATOM 3079 CH2 WAT S 89 ATOM 3070 CH2 WAT S 90 ATOM 3070 CH2 WAT S 90 ATOM 3070 CH2 WAT S 91 ATOM 3070 CH2 WAT S 91 ATOM 3080 CH2 WAT S 92 ATOM 3080 CH2 WAT S 93 ATOM 3080 CH2 WAT S 94 ATOM 3080 CH2 WAT S 95 ATOM 3080 CH2 WAT S 95 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 97 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 99 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 97 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 97 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 97 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 96 ATOM 3080 CH2 WAT S 97 ATOM 3080 CH2 WAT S 98 ATOM 3080 CH2 WAT S 100 ATOM 3090 CH2 | | 3064 | OH2 WAT S | 7 7 | 18.451 | 25.555 | | | |
| ATOM 3066 OH2 WAT S 80 23.571 13.292 69.937 1.00 35.45 8 ATOM 3067 OH2 WAT S 81 29.891 18.071 46.109 1.00 22.84 8 ATOM 3069 OH2 WAT S 82 12.886 42.723 75.807 1.00 35.31 8 ATOM 3070 OH2 WAT S 83 41.348 15.471 45.004 1.00 47.24 8 ATOM 3071 OH2 WAT S 84 41.348 15.471 45.004 1.00 49.67 8 ATOM 3072 OH2 WAT S 85 30.444 35.217 51.882 1.00 38.15 8 ATOM 3073 OH2 WAT S 86 5.217 40.817 61.244 1.00 19.51 8 ATOM 3073 OH2 WAT S 86 5.217 40.817 61.244 1.00 19.51 8 ATOM 3075 OH2 WAT S 88 41.816 25.022 72.452 1.00 22.92 8 ATOM 3076 OH2 WAT S 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3076 OH2 WAT S 89 50.621 36.644 60.248 1.00 30.72 8 ATOM 3077 OH2 WAT S 89 50.621 36.644 60.248 1.00 30.72 8 ATOM 3078 OH2 WAT S 90 26.008 34.532 49.627 1.00 45.42 8 ATOM 3079 OH2 WAT S 91 8.131 39.168 54.903 1.00 31.50 8 ATOM 3080 OH2 WAT S 93 34.773 54.065 69.382 1.00 36.05 8 ATOM 3080 OH2 WAT S 94 42.105 31.720 71.257 1.00 35.47 8 ATOM 3083 OH2 WAT S 95 26.641 37.426 38.934 1.00 31.50 8 ATOM 3083 OH2 WAT S 96 26.411 37.426 38.934 1.00 31.51 8 ATOM 3083 OH2 WAT S 98 25.060 18.985 36.669 1.00 46.63 8 ATOM 3085 OH2 WAT S 99 25.000 18.985 36.669 1.00 33.366 8 ATOM 3080 OH2 WAT S 99 25.000 18.985 36.669 1.00 46.63 8 ATOM 3080 OH2 WAT S 98 25.060 18.985 36.669 1.00 46.63 8 ATOM 3080 OH2 WAT S 100 37.304 39.027 73.722 1.00 35.77 8 ATOM 3080 OH2 WAT S 100 37.304 39.027 73.722 1.00 35.79 8 ATOM 3089 OH2 WAT S 100 37.304 39.027 73.722 1.00 35.79 8 ATOM 3089 OH2 WAT S 100 37.304 39.027 73.722 1.00 35.71 8 ATOM 3089 OH2 WAT S 100 37.304 39.027 73.722 1.00 35.71 8 ATOM 3089 OH2 WAT S 100 42.477 21.773 46.986 1.00 49.05 8 ATOM 3099 OH2 WAT S 100 42.297 74.111 1.00 25.23 8 ATOM 3099 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3099 OH2 WAT S 104 42.477 11.773 46.986 1.00 49.05 8 ATOM 3099 OH2 WAT S 104 42.477 11.773 46.986 1.00 49.05 8 ATOM 3099 OH2 WAT S 100 42.477 11.773 46.986 1.00 49.05 8 ATOM 3099 OH2 WAT S 101 42.4791 14.674 50.081 1.00 35.71 8 ATOM 3099 OH2 WAT S 103 42.4797 14.674 50.081 1.00 35.71 8 ATOM 3099 OH2 WAT S 104 42.4797 14.674 50.081 | | | OUR WAT S | 78 | 10.446 | 61 <i>.</i> 273 | 48.633 | 1.00 44.74 | |
| ATOM 3066 OH2 WAT S 80 ATOM 3068 CH2 WAT S 81 ATOM 3068 CH2 WAT S 81 ATOM 3068 CH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 82 ATOM 3071 OH2 WAT S 83 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 85 ATOM 3072 OH2 WAT S 85 ATOM 3072 OH2 WAT S 85 ATOM 3073 OH2 WAT S 85 ATOM 3074 OH2 WAT S 86 ATOM 3075 OH2 WAT S 87 ATOM 3076 OH2 WAT S 88 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 89 ATOM 3078 OH2 WAT S 90 ATOM 3079 OH2 WAT S 91 ATOM 3080 OH2 WAT S 91 ATOM 3080 OH2 WAT S 92 ATOM 3080 OH2 WAT S 94 ATOM 3081 OH2 WAT S 94 ATOM 3083 OH2 WAT S 95 ATOM 3083 OH2 WAT S 95 ATOM 3084 OH2 WAT S 96 ATOM 3085 OH2 WAT S 97 ATOM 3085 OH2 WAT S 98 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 94 ATOM 3080 OH2 WAT S 95 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 | ATOM | | UNZ WAT D | | | 24 051 | 73.017 | 1.00 35.45 | 8 |
| ATOM 3067 OH2 WAT S 80 ATOM 3068 CH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 82 ATOM 3070 OH2 WAT S 83 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 85 ATOM 3072 OH2 WAT S 85 ATOM 3073 OH2 WAT S 85 ATOM 3073 OH2 WAT S 86 ATOM 3074 CH2 WAT S 86 ATOM 3075 OH2 WAT S 87 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 88 ATOM 3077 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3077 OH2 WAT S 90 ATOM 3078 OH2 WAT S 91 ATOM 3079 OH2 WAT S 91 ATOM 3079 OH2 WAT S 92 ATOM 3080 OH2 WAT S 93 ATOM 3080 OH2 WAT S 93 ATOM 3080 OH2 WAT S 93 ATOM 3081 OH2 WAT S 94 ATOM 3081 OH2 WAT S 95 ATOM 3083 OH2 WAT S 96 ATOM 3084 OH2 WAT S 96 ATOM 3085 OH2 WAT S 97 ATOM 3085 OH2 WAT S 98 ATOM 3086 OH2 WAT S 98 ATOM 3086 OH2 WAT S 98 ATOM 3087 OH2 WAT S 99 ATOM 3088 OH2 WAT S 99 ATOM 3088 OH2 WAT S 99 ATOM 3089 OH2 WAT S 99 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 96 ATOM 3080 OH2 WAT S 97 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 98 ATOM 3080 OH2 WAT S 99 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 WAT S 110 ATOM 3090 | ATOM | 3066 | | | | | | | R |
| ATOM 3068 CH2 WAT S 81 ATOM 3069 OH2 WAT S 82 ATOM 3070 OH2 WAT S 82 ATOM 3071 OH2 WAT S 83 ATOM 3071 OH2 WAT S 84 ATOM 3071 OH2 WAT S 84 ATOM 3072 CH2 WAT S 85 ATOM 3072 OH2 WAT S 85 ATOM 3073 OH2 WAT S 85 ATOM 3074 CH2 WAT S 85 ATOM 3075 CH2 WAT S 87 ATOM 3075 CH2 WAT S 88 ATOM 3076 OH2 WAT S 88 ATOM 3077 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3077 OH2 WAT S 89 ATOM 3078 CH2 WAT S 90 ATOM 3078 OH2 WAT S 91 ATOM 3078 OH2 WAT S 91 ATOM 3080 OH2 WAT S 92 ATOM 3080 OH2 WAT S 92 ATOM 3081 CH2 WAT S 93 ATOM 3081 CH2 WAT S 94 ATOM 3081 CH2 WAT S 95 ATOM 3082 CH2 WAT S 95 ATOM 3083 OH2 WAT S 95 ATOM 3084 CH2 WAT S 98 ATOM 3085 CH2 WAT S 98 ATOM 3086 OH2 WAT S 98 ATOM 3087 OH2 WAT S 98 ATOM 3088 OH2 WAT S 98 ATOM 3088 OH2 WAT S 98 ATOM 3089 OH2 WAT S 98 ATOM 3089 OH2 WAT S 100 ATOM 3080 OH2 WAT S 102 ATOM 3080 OH2 WAT S 100 ATOM 3090 OH2 WAT S 110 ATOM 3090 OH2 W | MOTA | 3067 | OH2 WAT S | 80 | | | | | |
| ATOM 3069 OH2 WAT S 82 | | | OH2 WAT S | 81 | 29.891 | 18.071 | 46.109 | | |
| ATOM 3069 OH2 WAT S 83 | | | | | 12 886 | 42.723 | 75.807 | 1.00 35.31 | 8 |
| ATOM 3070 GH2 WAT S 84 ATOM 3071 GH2 WAT S 85 ATOM 3072 GH2 WAT S 85 ATOM 3073 GH2 WAT S 85 ATOM 3074 GH2 WAT S 86 ATOM 3074 GH2 WAT S 87 ATOM 3075 GH2 WAT S 88 ATOM 3075 GH2 WAT S 88 ATOM 3076 GH2 WAT S 88 ATOM 3076 GH2 WAT S 89 ATOM 3077 GH2 WAT S 89 ATOM 3077 GH2 WAT S 90 ATOM 3077 GH2 WAT S 90 ATOM 3078 GH2 WAT S 91 ATOM 3079 GH2 WAT S 92 ATOM 3079 GH2 WAT S 92 ATOM 3079 GH2 WAT S 92 ATOM 3080 GH2 WAT S 93 ATOM 3081 GH2 WAT S 94 ATOM 3082 GH2 WAT S 95 ATOM 3083 GH2 WAT S 95 ATOM 3083 GH2 WAT S 96 ATOM 3086 GH2 WAT S 97 ATOM 3086 GH2 WAT S 98 ATOM 3086 GH2 WAT S 99 ATOM 3086 GH2 WAT S 97 ATOM 3086 GH2 WAT S 98 ATOM 3086 GH2 WAT S 99 ATOM 3087 GH2 WAT S 100 ATOM 3088 GH2 WAT S 101 ATOM 3089 GH2 WAT S 102 ATOM 3080 GH2 WAT S 103 ATOM 3080 GH2 WAT S 104 ATOM 3080 GH2 WAT S 105 ATOM 3080 GH2 WAT S 105 ATOM 3080 GH2 WAT S 105 ATOM 3080 GH2 WAT S 106 ATOM 3080 GH2 WAT S 107 ATOM 3080 GH2 WAT S 108 ATOM 3080 GH2 WAT S 100 ATOM 3090 GH2 WAT S 110 ATOM 3090 | ATOM | 3069 | | | | | | 1 00 47 24 | 8 |
| ATOM 3071 OH2 WAT S 84 133.406 44.647 71.349 1.00 49.57 8 ATOM 3072 OH2 WAT S 85 30.444 35.217 51.882 1.00 30.72 8 ATOM 3073 OH2 WAT S 86 5.217 40.817 61.244 1.00 19.51 8 ATOM 3074 CH2 WAT S 87 8.891 21.532 56.838 1.00 30.72 8 ATOM 3075 OH2 WAT S 88 8.891 21.532 56.838 1.00 29.29 8 ATOM 3076 OH2 WAT S 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3077 OH2 WAT S 90 26.008 34.532 49.627 1.00 45.42 8 ATOM 3078 OH2 WAT S 91 8.131 39.168 54.903 1.00 31.50 8 ATOM 3079 OH2 WAT S 92 16.591 58.091 57.551 1.00 34.73 8 ATOM 3080 OH2 WAT S 93 34.773 54.065 69.382 1.00 36.05 8 ATOM 3081 OH2 WAT S 94 42.105 31.720 71.257 1.00 35.49 8 ATOM 3083 OH2 WAT S 95 26.411 37.426 38.934 1.00 41.68 8 ATOM 3085 OH2 WAT S 98 21.167 6.202 63.102 1.00 33.36 8 ATOM 3085 OH2 WAT S 98 21.167 6.202 63.102 1.00 33.36 8 ATOM 3086 OH2 WAT S 99 25.060 18.985 36.669 1.00 46.63 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3089 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3089 OH2 WAT S 102 48.730 25.803 59.572 1.00 37.97 8 ATOM 3090 OH2 WAT S 103 42.407 21.773 46.986 1.00 49.05 8 ATOM 3091 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3093 OH2 WAT S 106 9.750 32.487 48.823 1.00 37.97 8 ATOM 3094 OH2 WAT S 108 7.683 31.371 58.896 1.00 40.03 8 ATOM 3095 OH2 WAT S 108 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 100 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 100 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 100 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 100 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.683 31.371 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3099 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.08 8 ATOM 3099 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.08 8 ATOM 3099 OH2 WAT S 111 24.791 14.674 50.081 1.00 27.53 8 ATOM 3099 OH2 WAT S 111 24.791 14.674 50.081 1.00 27.53 8 ATOM 3099 OH2 WAT S 111 24.791 14.674 50.081 1.00 27.53 8 ATOM 3099 OH2 WAT S 112 24.791 14.674 | MOTA | 3070 | OH2 WAT S | 83 · | | | | | |
| ATOM 3072 | | - | | 84 | 13.406 | 44.647 | | | |
| ATOM 3072 | | | | 85 | 30.444 | 35,217 | 51.882 | | |
| ATOM 3073 OH2 WAT S 87 ATOM 3074 CH2 WAT S 88 ATOM 3075 OH2 WAT S 88 ATOM 3076 OH2 WAT S 89 ATOM 3076 OH2 WAT S 89 ATOM 3077 OH2 WAT S 90 ATOM 3077 OH2 WAT S 90 ATOM 3077 OH2 WAT S 91 ATOM 3079 OH2 WAT S 91 ATOM 3079 OH2 WAT S 92 ATOM 3080 OH2 WAT S 93 ATOM 3080 OH2 WAT S 94 ATOM 3081 OH2 WAT S 94 ATOM 3082 OH2 WAT S 95 ATOM 3083 OH2 WAT S 95 ATOM 3084 OH2 WAT S 97 ATOM 3085 OH2 WAT S 97 ATOM 3086 OH2 WAT S 97 ATOM 3086 OH2 WAT S 98 ATOM 3087 OH2 WAT S 99 ATOM 3088 OH2 WAT S 99 ATOM 3089 OH2 WAT S 100 ATOM 3089 OH2 WAT S 100 ATOM 3089 OH2 WAT S 101 ATOM 3089 OH2 WAT S 102 ATOM 3089 OH2 WAT S 103 ATOM 3089 OH2 WAT S 104 ATOM 3090 OH2 WAT S 105 ATOM 3091 OH2 WAT S 105 ATOM 3090 OH2 WAT S 106 ATOM 3091 OH2 WAT S 107 ATOM 3091 OH2 WAT S 107 ATOM 3091 OH2 WAT S 107 ATOM 3092 OH2 WAT S 107 ATOM 3093 OH2 WAT S 108 ATOM 3090 OH2 WAT S 107 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 105 ATOM 3090 OH2 WAT S 106 ATOM 3090 OH2 WAT S 107 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 107 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 107 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 106 ATOM 3090 OH2 WAT S 107 ATOM 3090 OH2 WAT S 108 ATOM 3090 OH2 WAT S 109 ATOM 3090 OH2 WAT S 110 ATOM 3090 OH2 WAT S 111 ATOM 3090 OH2 WAT S 111 ATOM 3090 OH2 WAT S 112 ATOM 3090 OH2 WAT S 113 ATOM 3090 OH2 WAT S 114 ATOM 3090 OH2 WAT S 116 ATOM 3090 OH2 WAT S 117 ATOM 3090 OH2 WAT S 117 ATOM 3090 OH2 WAT S 110 ATO | ATOM | 3072 | | | | | | 1.00 19.51 | 8 |
| ATOM 3075 CH2 WAT S 87 ATOM 3075 CH2 WAT S 88 ATOM 3076 CH2 WAT S 89 ATOM 3076 CH2 WAT S 89 ATOM 3077 CH2 WAT S 90 ATOM 3077 CH2 WAT S 90 ATOM 3078 CH2 WAT S 91 ATOM 3079 CH2 WAT S 92 ATOM 3080 CH2 WAT S 92 ATOM 3081 CH2 WAT S 93 ATOM 3082 CH2 WAT S 94 ATOM 3082 CH2 WAT S 95 ATOM 3083 CH2 WAT S 95 ATOM 3083 CH2 WAT S 96 ATOM 3084 CH2 WAT S 97 ATOM 3085 CH2 WAT S 97 ATOM 3086 CH2 WAT S 97 ATOM 3088 CH2 WAT S 98 ATOM 3089 CH2 WAT S 100 ATOM 3089 CH2 WAT S 101 ATOM 3089 CH2 WAT S 101 ATOM 3089 CH2 WAT S 102 ATOM 3089 CH2 WAT S 102 ATOM 3089 CH2 WAT S 103 ATOM 3089 CH2 WAT S 104 ATOM 3099 CH2 WAT S 105 ATOM 3090 CH2 WAT S 106 ATOM 3093 CH2 WAT S 107 ATOM 3093 CH2 WAT S 108 ATOM 3093 CH2 WAT S 108 ATOM 3094 CH2 WAT S 108 ATOM 3095 CH2 WAT S 108 ATOM 3095 CH2 WAT S 108 ATOM 3097 CH2 WAT S 108 ATOM 3099 CH2 WAT S 110 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 110 ATOM | ATOM | 3073 | | | | | | | |
| ATOM 3075 OH2 WAT S 88 50.621 36.644 60.248 1.00 29.29 8 ATOM 3076 OH2 WAT S 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3077 OH2 WAT S 90 26.008 34.532 49.627 1.00 45.42 8 ATOM 3078 OH2 WAT S 91 8.131 39.168 54.903 1.00 31.50 8 ATOM 3079 OH2 WAT S 92 16.591 58.091 57.551 1.00 34.73 8 ATOM 3080 OH2 WAT S 93 34.773 54.065 69.382 1.00 36.05 8 ATOM 3081 OH2 WAT S 94 42.105 31.720 71.257 1.00 35.49 8 ATOM 3082 OH2 WAT S 95 29.684 52.077 73.172 1.00 35.17 8 ATOM 3083 OH2 WAT S 96 26.411 37.426 38.934 1.00 41.68 8 ATOM 3084 OH2 WAT S 97 41.183 52.989 62.927 1.00 50.77 8 ATOM 3085 OH2 WAT S 98 21.167 6.202 63.102 1.00 33.36 8 ATOM 3086 OH2 WAT S 99 25.060 18.985 36.669 1.00 46.63 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 29.88 8 ATOM 3089 OH2 WAT S 102 48.730 25.803 59.572 1.00 37.97 8 ATOM 3090 OH2 WAT S 103 24.029 42.997 74.111 1.00 25.23 8 ATOM 3091 OH2 WAT S 105 40.850 36.936 1.00 49.05 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 1.885 1.00 44.21 8 ATOM 3094 OH2 WAT S 107 9.750 32.487 48.823 1.00 35.71 8 ATOM 3095 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3097 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 110 40.750 47.494 54.056 1.00 34.08 8 ATOM 3099 OH2 WAT S 112 44.791 14.674 50.081 1.00 51.96 8 ATOM 3099 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3099 OH2 WAT S 114 7.708 42.479 57.566 1.00 34.08 8 ATOM 3099 OH2 WAT S 114 7.708 42.479 77.566 1.00 27.53 8 | | 3074 | CH2 WAT S | 87 | 8.891 | | | | |
| ATOM 3076 OH2 WAT S 89 50.621 36.644 60.248 1.00 29.29 8 ATOM 3077 OH2 WAT S 90 26.008 34.532 49.627 1.00 45.42 ATOM 3078 OH2 WAT S 91 8.131 39.168 54.903 1.00 31.50 8 ATOM 3079 OH2 WAT S 92 16.591 58.091 57.551 1.00 34.73 8 ATOM 3080 OH2 WAT S 94 42.105 31.720 71.257 1.00 35.49 8 ATOM 3081 OH2 WAT S 95 29.684 52.077 73.172 1.00 35.17 8 ATOM 3083 OH2 WAT S 96 26.411 37.426 38.934 1.00 41.68 8 ATOM 3084 OH2 WAT S 98 21.167 6.202 63.102 1.00 33.36 8 ATOM 3085 OH2 WAT S 98 25.060 18.985 36.669 1.00 46.63 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3089 OH2 WAT S 101 15.911 54.635 39.343 1.00 29.88 8 ATOM 3090 OH2 WAT S 103 42.4029 42.997 74.111 1.00 25.23 8 ATOM 3090 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3093 OH2 WAT S 105 24.029 42.997 74.111 1.00 25.23 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 49.05 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 49.05 8 ATOM 3094 OH2 WAT S 106 40.850 36.936 31.885 1.00 49.05 8 ATOM 3095 OH2 WAT S 106 40.850 36.936 31.885 1.00 40.03 8 ATOM 3095 OH2 WAT S 106 40.850 36.936 31.885 1.00 40.03 8 ATOM 3095 OH2 WAT S 106 40.850 36.936 31.885 1.00 40.03 8 ATOM 3095 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3095 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3097 OH2 WAT S 106 40.850 36.936 31.885 1.00 35.71 8 ATOM 3098 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3099 OH2 WAT S 110 40.750 47.494 54.056 1.00 30.02 8 ATOM 3099 OH2 WAT S 111 40.750 47.494 54.056 1.00 46.98 8 ATOM 3099 OH2 WAT S 112 44.791 14.674 50.081 1.00 31.00 51.96 8 ATOM 3099 OH2 WAT S 112 44.791 14.674 50.081 1.00 31.00 51.96 8 ATOM 3099 OH2 WAT S 112 44.791 14.674 50.081 1.00 27.53 8 | | | | 88 | 41.816 | 25.022 | 72.452 | | |
| ATOM 3076 OH2 WAT S 90 26.008 34.532 49.627 1.00 45.42 8 ATOM 3077 OH2 WAT S 91 8.131 39.168 54.903 1.00 31.50 8 ATOM 3079 OH2 WAT S 92 16.591 58.091 57.551 1.00 34.73 8 ATOM 3080 OH2 WAT S 93 34.773 54.065 69.382 1.00 36.05 8 ATOM 3081 OH2 WAT S 94 42.105 31.720 71.257 1.00 35.49 8 ATOM 3082 OH2 WAT S 95 29.684 52.077 73.172 1.00 35.17 8 ATOM 3083 OH2 WAT S 96 26.411 37.426 38.934 1.00 41.68 8 ATOM 3083 OH2 WAT S 97 41.183 52.989 62.927 1.00 50.77 8 ATOM 3085 OH2 WAT S 98 21.167 6.202 63.102 1.00 33.36 8 ATOM 3086 OH2 WAT S 99 25.060 18.985 36.669 1.00 46.63 8 ATOM 3087 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3088 OH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3089 OH2 WAT S 101 15.911 54.635 39.343 1.00 29.88 8 ATOM 3089 OH2 WAT S 102 48.730 25.803 59.572 1.00 37.97 8 ATOM 3090 OH2 WAT S 103 24.029 42.997 74.111 1.00 25.23 8 ATOM 3091 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3093 OH2 WAT S 105 29.984 22.945 31.397 1.00 44.21 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3095 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3097 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3099 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3099 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3099 OH2 WAT S 111 22.590 8.744 67.501 1.00 34.08 8 ATOM 3099 OH2 WAT S 111 22.590 8.744 67.501 1.00 34.08 8 ATOM 3099 OH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3099 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3099 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3099 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3091 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3091 OH2 WAT S 113 40.750 47.494 | ATOM | | ••••• | | | | 60.248 | 1.00 29.29 | 8 |
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| ATOM 3078 | | 3077 | OH2 WAT S | 90 | 25.008 | | | | |
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| ATOM 3082 CH2 WAT S 96 ATOM 3083 OH2 WAT S 96 ATOM 3084 OH2 WAT S 97 ATOM 3085 OH2 WAT S 98 ATOM 3085 OH2 WAT S 98 ATOM 3086 OH2 WAT S 99 ATOM 3087 OH2 WAT S 100 ATOM 3088 OH2 WAT S 101 ATOM 3089 OH2 WAT S 101 ATOM 3089 OH2 WAT S 102 ATOM 3090 OH2 WAT S 103 ATOM 3090 OH2 WAT S 104 ATOM 3091 OH2 WAT S 105 ATOM 3092 OH2 WAT S 105 ATOM 3093 OH2 WAT S 106 ATOM 3093 OH2 WAT S 106 ATOM 3094 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3095 OH2 WAT S 107 ATOM 3096 OH2 WAT S 108 ATOM 3097 OH2 WAT S 108 ATOM 3090 OH2 WAT S 106 ATOM 3090 OH2 WAT S 106 ATOM 3091 OH2 WAT S 106 ATOM 3093 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 109 ATOM 3098 OH2 WAT S 110 ATOM 3098 OH2 WAT S 111 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3100 OH2 WAT S 113 ATOM 3100 OH2 WAT S 113 ATOM 3100 OH2 WAT S 114 ATOM 3101 OH2 WAT S 114 ATOM 3101 OH2 WAT S 113 ATOM 3100 OH2 WAT S 114 ATOM 3101 OH2 WAT S 113 ATOM 3101 OH2 WAT S 114 ATOM 3101 OH | | | | | 29 684 | 52 077 | 73.172 | 1.00 35.17 | 8 |
| ATOM 3083 GH2 WAT S 96 ATOM 3084 GH2 WAT S 97 ATOM 3085 GH2 WAT S 98 ATOM 3085 GH2 WAT S 98 ATOM 3086 GH2 WAT S 99 ATOM 3087 OH2 WAT S 100 ATOM 3088 GH2 WAT S 101 ATOM 3088 GH2 WAT S 101 ATOM 3089 GH2 WAT S 101 ATOM 3090 GH2 WAT S 102 ATOM 3091 GH2 WAT S 105 ATOM 3092 GH2 WAT S 105 ATOM 3093 GH2 WAT S 106 ATOM 3093 GH2 WAT S 106 ATOM 3094 GH2 WAT S 107 ATOM 3095 GH2 WAT S 108 ATOM 3095 GH2 WAT S 108 ATOM 3096 GH2 WAT S 108 ATOM 3097 GH2 WAT S 108 ATOM 3098 GH2 WAT S 106 ATOM 3099 GH2 WAT S 107 ATOM 3094 GH2 WAT S 108 ATOM 3095 GH2 WAT S 108 ATOM 3095 GH2 WAT S 108 ATOM 3096 GH2 WAT S 108 ATOM 3097 GH2 WAT S 109 ATOM 3097 GH2 WAT S 108 ATOM 3098 GH2 WAT S 109 ATOM 3096 GH2 WAT S 109 ATOM 3097 GH2 WAT S 108 ATOM 3098 GH2 WAT S 110 ATOM 3098 GH2 WAT S 110 ATOM 3099 GH2 WAT S 111 ATOM 3099 GH2 WAT S 112 ATOM 3099 GH2 WAT S 113 ATOM 3099 GH2 WAT S 114 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 113 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 114 ATOM 3100 GH2 WAT S 115 ATOM 3100 GH2 WAT S 116 ATOM 3095 GH2 WAT S 116 ATOM 3095 GH2 WAT S 116 ATOM 3096 G | MOTA | 3082 | | | | | | | 8 |
| ATOM 3084 OH2 WAT S 97 ATOM 3085 OH2 WAT S 98 ATOM 3086 OH2 WAT S 99 ATOM 3087 OH2 WAT S 100 ATOM 3088 OH2 WAT S 101 ATOM 3088 OH2 WAT S 101 ATOM 3089 OH2 WAT S 102 ATOM 3090 OH2 WAT S 103 ATOM 3091 OH2 WAT S 104 ATOM 3092 OH2 WAT S 105 ATOM 3093 OH2 WAT S 105 ATOM 3093 OH2 WAT S 106 ATOM 3094 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 109 ATOM 3098 OH2 WAT S 109 ATOM 3099 OH2 WAT S 108 ATOM 3090 OH2 WAT S 106 ATOM 3091 OH2 WAT S 107 ATOM 3094 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 109 ATOM 3098 OH2 WAT S 110 ATOM 3098 OH2 WAT S 110 ATOM 3099 OH2 WAT S 110 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 115 ATOM 3099 OH2 WAT S 116 ATOM 3099 OH2 WAT S 117 ATOM 3099 OH2 WAT S 118 ATOM 3099 OH2 WAT S 119 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 115 ATOM 3099 OH2 WAT S 116 ATOM 3099 OH2 WAT S 117 ATOM 3099 OH2 WAT S 118 ATOM 3099 OH2 WAT S 119 ATOM 3099 OH2 WAT S 110 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3090 OH2 WAT S 113 ATOM 3090 OH2 WAT S 113 ATOM 3090 OH2 WAT S 114 ATOM 3090 OH2 WAT S 113 ATOM 3090 OH2 WAT S 113 ATOM 3090 OH2 WAT S 114 ATOM 3090 OH2 WAT S 114 ATOM 3090 OH2 WAT S 116 ATOM 3090 OH2 WAT S 117 ATOM 3090 OH2 WAT S 110 ATOM 3090 OH2 WAT S 100 ATOM 3090 | MOTE | 3083 | OH2 WAT S | 96 | | | | | |
| ATOM 3085 CH2 WAT S 98 ATOM 3086 CH2 WAT S 99 ATOM 3087 CH2 WAT S 100 ATOM 3088 CH2 WAT S 100 ATOM 3088 CH2 WAT S 101 ATOM 3088 CH2 WAT S 101 ATOM 3089 CH2 WAT S 102 ATOM 3090 CH2 WAT S 103 ATOM 3091 CH2 WAT S 104 ATOM 3092 CH2 WAT S 105 ATOM 3093 CH2 WAT S 106 ATOM 3093 CH2 WAT S 107 ATOM 3094 CH2 WAT S 108 ATOM 3095 CH2 WAT S 108 ATOM 3096 CH2 WAT S 108 ATOM 3097 CH2 WAT S 109 ATOM 3098 CH2 WAT S 110 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 115 ATOM 3099 CH2 WAT S 116 ATOM 3099 CH2 WAT S 117 ATOM 3099 CH2 WAT S 118 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 115 ATOM 3099 CH2 WAT S 116 ATOM 3099 CH2 WAT S 117 ATOM 3099 CH2 WAT S 117 ATOM 3099 CH2 WAT S 118 ATOM 3099 CH2 WAT S 118 ATOM 3099 CH2 WAT S 119 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 113 ATOM 3090 CH2 WAT S 114 ATOM 3090 CH2 WAT S 100 ATOM 3090 CH2 WAT S 100 ATOM 3090 CH2 WAT S 100 ATOM 309 | | | OH2 WAT S | 97 | 41.183 | 52.989 | | | |
| ATOM 3085 CH2 WAT S 99 ATOM 3086 CH2 WAT S 99 ATOM 3087 OH2 WAT S 100 ATOM 3087 OH2 WAT S 100 ATOM 3088 CH2 WAT S 101 ATOM 3088 CH2 WAT S 101 ATOM 3089 CH2 WAT S 101 ATOM 3090 CH2 WAT S 103 ATOM 3091 OH2 WAT S 104 ATOM 3092 CH2 WAT S 105 ATOM 3092 CH2 WAT S 105 ATOM 3093 CH2 WAT S 106 ATOM 3094 CH2 WAT S 107 ATOM 3095 CH2 WAT S 108 ATOM 3096 CH2 WAT S 108 ATOM 3096 CH2 WAT S 109 ATOM 3097 CH2 WAT S 109 ATOM 3098 CH2 WAT S 110 ATOM 3099 CH2 WAT S 110 ATOM 3099 CH2 WAT S 110 ATOM 3096 CH2 WAT S 110 ATOM 3097 CH2 WAT S 110 ATOM 3098 CH2 WAT S 110 ATOM 3099 CH2 WAT S 110 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 115 ATOM 3099 CH2 WAT S 116 ATOM 3099 CH2 WAT S 117 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 115 ATOM 3099 CH2 WAT S 116 ATOM 3099 CH2 WAT S 117 ATOM 3090 CH2 WAT S 100 ATOM 3090 CH2 WAT S 100 ATOM 309 | | | | | | 6.202 | 63.102 | 1.00 33.36 | 8 |
| ATOM 3086 SH2 WAT S 100 37.304 39.027 73.722 1.00 25.99 8 ATOM 3088 SH2 WAT S 101 15.911 54.635 39.343 1.00 29.88 8 ATOM 3089 SH2 WAT S 102 48.730 25.803 59.572 1.00 37.97 8 ATOM 3090 SH2 WAT S 103 24.029 42.997 74.111 1.00 25.23 8 ATOM 3091 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3092 SH2 WAT S 105 29.984 22.945 31.397 1.00 44.21 8 ATOM 3093 SH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3094 SH2 WAT S 107 9.750 32.487 48.823 1.00 35.71 8 ATOM 3095 SH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3096 SH2 WAT S 109 17.603 13.771 59.767 1.00 50.33 8 ATOM 3096 SH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3098 SH2 WAT S 111 22.590 8.744 67.501 1.00 34.81 8 ATOM 3099 SH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3099 SH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3100 SH2 WAT S 113 40.750 47.494 54.056 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 SH2 WAT S 114 7.708 42.479 7.566 1.00 27.53 | ATOM | 3085 | CHZ WAT 5 | | | | | | 8 |
| ATOM 3087 OH2 WAT S 100 37.304 39.027 73.722 1.00 29.88 8 ATOM 3088 OH2 WAT S 101 15.911 54.635 39.343 1.00 29.88 8 ATOM 3089 OH2 WAT S 102 48.730 25.803 59.572 1.00 37.97 8 ATOM 3090 OH2 WAT S 103 24.029 42.997 74.111 1.00 25.23 8 ATOM 3091 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 ATOM 3092 OH2 WAT S 105 29.984 22.945 31.397 1.00 44.21 8 ATOM 3093 OH2 WAT S 106 40.850 36.936 31.885 1.00 43.26 8 ATOM 3094 OH2 WAT S 107 9.750 32.487 48.823 1.00 35.71 8 ATOM 3095 OH2 WAT S 108 7.618 30.171 59.767 1.00 50.33 8 ATOM 3096 OH2 WAT S 109 17.603 13.771 59.767 1.00 50.33 8 ATOM 3097 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3098 OH2 WAT S 111 21.034 29.771 76.056 1.00 30.02 8 ATOM 3099 OH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3100 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 | MOTE | 3086 | OH2 WAT S | 99 | | | | | |
| ATOM 3088 CH2 WAT S 101 | | | OF WAT S | 100 . | 37.304 | 39.027 | 73.722 | | |
| ATOM 3088 SH2 WAT S 101 | ATOM | | U112 1177 5 | 101 | 15 011 | 54 635 | 39.343 | 1.00 29.88 | .8 |
| ATOM 3089 CH2 WAT S 102 ATOM 3090 CH2 WAT S 103 ATOM 3091 CH2 WAT S 104 ATOM 3092 CH2 WAT S 105 ATOM 3093 CH2 WAT S 106 ATOM 3093 CH2 WAT S 106 ATOM 3094 CH2 WAT S 107 ATOM 3095 CH2 WAT S 107 ATOM 3095 CH2 WAT S 108 ATOM 3096 CH2 WAT S 108 ATOM 3096 CH2 WAT S 109 ATOM 3097 CH2 WAT S 109 ATOM 3098 CH2 WAT S 110 ATOM 3098 CH2 WAT S 111 ATOM 3098 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3099 CH2 WAT S 115 ATOM 3099 CH2 WAT S 116 ATOM 3099 CH2 WAT S 117 ATOM 3099 CH2 WAT S 118 ATOM 3099 CH2 WAT S 119 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3099 CH2 WAT S 114 ATOM 3100 CH2 WAT S 114 ATOM 3 | MOTA | 3088 | CH2 WAT S | TUL | | | | | 8 |
| ATOM 3090 OH2 WAT S 103 ATOM 3091 OH2 WAT S 104 ATOM 3092 OH2 WAT S 105 ATOM 3093 OH2 WAT S 106 ATOM 3093 OH2 WAT S 106 ATOM 3094 OH2 WAT S 107 ATOM 3095 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 110 ATOM 3098 OH2 WAT S 111 ATOM 3098 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3099 OH2 WAT S 115 ATOM 3099 OH2 WAT S 116 ATOM 3099 OH2 WAT S 117 ATOM 3099 OH2 WAT S 118 ATOM 3099 OH2 WAT S 119 ATOM 3100 OH2 WAT S 113 ATOM 3100 OH2 WAT S 114 | | 3089 | CH2 WAT S | 102 | 48.730 | | | | |
| ATOM 3091 OH2 WAT S 104 42.477 21.773 46.986 1.00 49.05 8 40.00 40 40.00 | | | AND WATER | 103 | 24.029 | 42.997 | 74.111 | | |
| ATOM 3091 OH2 WAT S 104 | | | JRZ WAT S | 104 | | | 46.986 | 1.00 49.05 | 8 |
| ATOM 3092 OH2 WAT S 105 ATOM 3093 OH2 WAT S 106 ATOM 3094 OH2 WAT S 107 ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 109 ATOM 3097 OH2 WAT S 110 ATOM 3098 OH2 WAT S 111 ATOM 3098 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 112 ATOM 3099 OH2 WAT S 113 ATOM 3099 OH2 WAT S 114 ATOM 3100 OH2 WAT S 113 ATOM 3100 OH2 WAT S 114 ATOM 3100 OH2 WAT S 114 ATOM 3101 OH2 WAT S 114 ATOM 3175 48 136 ATOM 3175 AR 136 | MOTA | 3091 | OH2 WAT S | 104 | | | | | 8 |
| ATOM 3093 CH2 WAT S 106 ATOM 3094 CH2 WAT S 107 ATOM 3095 CH2 WAT S 108 ATOM 3096 CH2 WAT S 108 ATOM 3096 CH2 WAT S 109 ATOM 3097 CH2 WAT S 110 ATOM 3098 CH2 WAT S 110 ATOM 3098 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 113 ATOM 3100 CH2 WAT S 113 ATOM 3100 CH2 WAT S 114 ATOM 3 | | | OH2 WAT S | 105 | | | | | |
| ATOM 3094 OH2 WAT S 107 9.750 32.487 48.823 1.00 35.71 8 ATOM 3095 OH2 WAT S 108 7.618 30.171 58.896 1.00 40.03 8 ATOM 3096 OH2 WAT S 109 17.603 13.771 59.767 1.00 50.33 8 ATOM 3097 OH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3098 OH2 WAT S 111 21.034 29.771 76.056 1.00 30.02 8 ATOM 3099 OH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3100 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 77.566 1.00 27.53 8 | | | ב תבנו כאם | 106 | 40.850 | 36.936 | | | 0 |
| ATOM 3094 CH2 WAT S 108 ATOM 3095 CH2 WAT S 108 ATOM 3096 CH2 WAT S 109 ATOM 3096 CH2 WAT S 109 ATOM 3097 CH2 WAT S 110 ATOM 3097 CH2 WAT S 110 ATOM 3098 CH2 WAT S 111 ATOM 3098 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3099 CH2 WAT S 112 ATOM 3100 CH2 WAT S 113 ATOM 3100 CH2 WAT S 113 ATOM 3100 CH2 WAT S 114 ATOM 3101 CH2 WAT S 115 | | | OHE HAL S | 107 | | | | 1.00 35.71 | |
| ATOM 3095 OH2 WAT S 108 ATOM 3096 OH2 WAT S 109 ATOM 3097 OH2 WAT S 110 ATOM 3097 OH2 WAT S 110 ATOM 3098 OH2 WAT S 111 ATOM 3099 OH2 WAT S 111 ATOM 3099 OH2 WAT S 112 ATOM 3100 OH2 WAT S 113 ATOM 3100 OH2 WAT S 113 ATOM 3101 OH2 WAT S 114 | ATOM | 3094 | OH2 WAT S | 10/ | | | | | |
| ATOM 3096 CH2 WAT S 109 ATOM 3097 CH2 WAT S 110 ATOM 3098 CH2 WAT S 111 ATOM 3098 CH2 WAT S 111 ATOM 3099 CH2 WAT S 111 ATOM 3099 CH2 WAT S 112 ATOM 3100 CH2 WAT S 113 ATOM 3100 CH2 WAT S 114 ATOM 3101 CH2 WAT S 114 ATOM 3 | | | CH2 WAT S | 108 | | | | | |
| ATOM 3096 CH2 WAT S 110 22.590 8.744 67.501 1.00 34.81 8 ATOM 3097 CH2 WAT S 110 22.590 8.744 67.501 1.00 30.02 8 ATOM 3098 CH2 WAT S 111 21.034 29.771 76.056 1.00 30.02 8 ATOM 3099 CH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3100 CH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 CH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 CH2 WAT S 114 7.708 42.479 77.566 1.00 27.53 8 | | | ב מדעון כער | 109 | 17.603 | 13.771 | 59.767 | 1.00 50.33 | |
| ATOM 3097 SH2 WAT S 110 ATOM 3098 SH2 WAT S 111 ATOM 3099 SH2 WAT S 111 ATOM 3099 SH2 WAT S 112 ATOM 3100 SH2 WAT S 113 ATOM 3100 SH2 WAT S 113 ATOM 3101 SH2 WAT S 114 ATOM 3101 SH2 WAT S 115 ATOM 3101 SH2 WAT S 1 | atom | | UNZ WAI 5 | 110 | | | | 1.00 34.81 | 8 |
| ATOM 3098 CH2 WAT S 111 21.034 29.771 76.036 1.00 51.96 8 ATOM 3099 CH2 WAT S 112 24.791 14.674 50.081 1.00 51.96 8 ATOM 3100 CH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 CH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 7.708 3101 CH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.479 1.00 34.08 8 7.708 42.408 1.00 34.08 8 7.708 8 7.708 8 7.708 8 7.708 8 7.708 8 7.708 8 7 | ATOM | 3097 | CH2 WAT S | 110 | | | | | 8 |
| ATOM 3099 OH2 WAT S 112 24.791 14.674 50.061 1.00 32.50 8 ATOM 3100 OH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 27.53 8 | | | CH2 WAT S | 111 | | | | . 00 51 05 | |
| ATOM 300 CH2 WAT S 113 40.750 47.494 54.056 1.00 46.98 8 ATOM 3101 CH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 CH2 WAT S 114 7.708 42.479 58.027 1.00 27.53 8 | | | | 112 | 24.791 | 14.674 | | | |
| ATON 3100 CH2 WAT S 114 7.708 42.479 58.027 1.00 34.08 8 ATOM 3101 OH2 WAT S 114 7.708 42.479 58.027 1.00 27.53 8 | | | | 113 | | | - 4 0 - 4 | 1.00 46.98 | |
| ATOM 3101 OH2 WAT 5 114 22 375 48 136 77.566 1.00 27.53 8 | ATOM | | | 2.2.4 | | | | 1.00 34.08 | 8 |
| 20 275 /0 126 11.000 1.00 27.33 | | 3101 | OHZ WAT S | 114 | | | | | |
| | | | | 115 | 32.375 | 49.136 | 11.300 | 1.00 200 | |

| | 2202 | OH2 WAT S 116 | | 5.596 | 17.009 | 64.551 | 1.00 39.15 | 8 |
|--------------|--------------|--------------------------------|---|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 3103 3104 | OH2 WAT S 117 | | 20.194 | 5.0.998 | 70.563 | 1.00 19.73 | 8 |
| ATOM ATOM | 3105 | OH2 WAT S 118 | | 23.853 | 64.927 | 64.164 | 1.00 27.16 | 8 8 |
| ATOM | 3106 | OH2 WAT S 119 | | 9.277 | 43.601 | 46.279 | 1.00 32.31 1.00 55.20 | 8 |
| ATOM | 3107 | OH2 WAT S 120 | | 15.613 | 24.398 | 46.723 | 1.00 35.20 | 8 |
| ATOM | 3108 | OH2 WAT S 121 | | 33.110 | 16.122 | 54.229 33.852 | 1.00 37.49 | 8 |
| ATOM | 3109 | OH2 WAT S 122 | | 26.772 | 34.085 | 75.829 | 1.00 47.30 | 8 |
| ATOM | 3110 | OH2 WAT S 123 | | 28.654 | 37.783 22.653 | 59.678 | 1.00 37.33 | 8 |
| ATOM | 3111 | OH2 WAT S 124 | | 49.180 | 27.788 | 65.975 | 1.00 67.86 | 8 |
| MOTA | 3112 | OH2 WAT S 125 | | 20.561 34.251 | 13.344 | 57.366 | 1.00 36.18 | 8 |
| MOTA | 3113 | OH2 WAT. 5 126 | | 49.215 | 36.854 | 48.117 | 1.00 33.63 | 8 |
| ATOM | 3114 | OH2 WAT S 127 OH2 WAT S 128 | | 45.826 | 19.588 | 41.601 | 1.00 44.07 | 8 |
| MOTA | 3115 | | | 18.693 | 56.382 | 64.014 | 1.00 47.77 | 8 . |
| MOTA | 3116 | OH2 WAT S 129 OH2 WAT S 130 | | 44.181 | 24.202 | 36.963 | 1.00 32.70 | 8 |
| ATOM | 3117 3118 | OH2 WAT S 131 | | 19.160 | 51.901 | 38.133 | 1.00 54.07 | 8 |
| ATOM | 3119 | OH2 WAT S 132 | | 16.904 | 36.558 | 48.679 | 1.00 42.21 | 8 8 |
| ATOM ATOM | 3120 | OH2 WAT 5 133 | | 46.851 | 26.029 | 34.353 | 1.00 56.33 1.00 45.99 | 8 |
| ATOM | 3121 | OH2 WAT S 134 | | 3.925 | 41.533 | 68.647 | 1.00 44.50 | 8 |
| ATOM | 3122 | OH2 WAT S 135 | | 44.590 | 38.382 | 78.167 71.166 | 1.00 28.17 | 8 |
| ATOM | 3123 | OH2 WAT S 136 | | 6.384 17.982 | 19.317 39.823 | 66.487 | 1.00 49.31 | 8 |
| MOTA | 3124 | OH2 WAT S 137 | | 8.317 | 22.286 | 61.863 | 1.00 43.42 | 8 |
| MOTA | 3125 | OH2 WAT S 138 | | 29.248 | 14.196 | 55.622 | 1.00 35.55 | 8 |
| ATOM | 3126 | OH2 WAT S 139 OH2 WAT S 140 | | 30.377 | 33.180 | 80.320 | 1.00 43.94 | 8 |
| MOTA | 3127 | | | 41.842 | 32.906 | 27.392 | 1.00 24.82 | 8 |
| MOTA | 3128 | OH2 WAT S 141 OH2 WAT S 142 | | 33.971 | 3.859 | 64.002 | 1.00 41.93 | 8 |
| MOTA | 3129 3130 | OH2 WAT S 143 | | 27.314 | 8.087 | 70.916 | 1.00 49.03 | 8 |
| ATOM ATOM | 3131 | OH2 WAT S 144 | | 4.310 | 39.006 | 64.550 | 1.00 32.70 | 8 8 |
| ATOM | 3132 | OH2 WAT S 145 | | 2.940 | 19.950 | 63.265 | 1.00 33.24 1.00 44.24 | 8 |
| ATOM | 3133 | OH2 WAT 5 146 | | 24.134 | 47.625 | 60.121 42.337 | 1.00 47.82 | 8 |
| ATOM | 3134 | OH2 WAT S 147 | | 25.035 | 53.746 38.897 | | 1.00 21.86 | 8 |
| ATOM | 3135 | OH2 WAT S 148 | | 32.767 | 57.288 | 47.392 | 1.00 36.13 | 8 |
| ATOM | 3136 | OH2 WAT 5 149 | | 37.145 25.171 | 18.011 | 32.273 | 1.00 38.04 | 8 |
| MOTA | 3137 | OH2 WAT S 150 OH2 WAT S 151 | | 24.054 | 43.182 | 55.583 | 1.00 41.68 | 8 |
| ATOM | 3138 | OH2 WAT S 151 OH2 WAT S 152 | | 27.686 | 64.936 | 52.937 | 1.00 60.62 | 8 |
| ATOM | 3139 3140 | OH2 WAT S 153 | | 24.084 | 39.543 | 76.589 | 1.00 22.62 | 8 |
| MOTA | 3141 | OH2 WAT S 154 | | 42.110 | 10.159 | 68.662 | 1.00 46.98 | 8 8 |
| MOTA MOTA | 3142 | OH2 WAT S 155 | | 9.675 | 22.905 | 75.335 | 1.00 26.45 1.00 33.84 | 8 |
| ATOM | 3143 | OH2 WAT 5 156 | | 4.506 | 34.799 | 52.857 76.446 | 1.00 35.34 | 8 |
| MOTA | 3144 | OH2 WAT S 157 | | 32.583 | 35.051 58.311 | 60.390 | 1.00 54.69 | 8 |
| ATOM | 3145 | OH2 WAT 5 158 | | 40.341 29.473 | 58.378 | 71.881 | 1.00 28.59 | 8 |
| MOTA | 3146 | OH2 WAT S 159 | | 11.829 | 60.543 | 56.138 | 1.00 37.67 | 8 |
| MOTA | 3147 | OH2 WAT S 160 | | 24.247 | | 67.935 | 1.00 56.62 | 8 |
| ATOM | 3148 | OH2 WAT S 161 OH2 WAT S 162 | | 12.853 | 33.929 | 77.503 | 1.00 29.88 | 8 |
| MOTA | 3149 | OH2 WAT 5 163 | | 9.49 | 26.168 | 59.687 | 1.00 15.42 | 8 |
| ATOM | 3150 3151 | OH2 WAT S 164 | | 27.424 | 16.480 | | 1.00 36.86 | 8 |
| MOTA MOTA | 3152 | OH2 WAT S 165 | | 8.512 | | | 1.00 30.08 1.00 39.47 | 8 |
| ATOM | 3153 | OH2 WAT S 166 | | 30.721 | | | | 8 |
| MOTA | 3154 | OH2 WAT S 167 | | 49.594 | | | | 8 |
| MOTA | 3155 | OH2 WAT S 168 | | 41.994 | | | | 8 |
| ATOM | 3156 | OH2 WAT S 169 | | 42.092 | | | | 8 |
| ATOM | 3157 | OH2 WAT S 170 | | 34.547 15.377 | | | | 8 |
| ATCM | 3158 | | | 31.854 | | | 1.00 42.43 | 8 |
| MOTA | 3159 | OH2 WAT S 172 | | 48.743 | | | 1.00 34.04 | 8 |
| ATOM | 3160 | OH2 WAT S 173 | | 8.723 | | | 1.00 32.87 | 8 |
| MOTA | 3161 | | | 14.257 | | 53.455 | | 8 |
| ATOM | 3162 | ~ . | | 31.917 | | 53.943 | 1.00 40.43 | 8 |
| ATOM | 3163 3164 | | | 23.921 | 47.029 | 70.642 | | 8 8 |
| MOTA MOTA | | 170 | | 27.974 | 47.778 | 69.949 | | 8 |
| MOTA MOTA | | OH2 WAT S 179 | | 7.850 | | | | 8 |
| ATOM | | OH2 WAT S 180 | | 22.080 | | | | |
| ATOM | | 101 | | 34.780 | 48.220 | , //.41; - | , 1.00 50.00 | • |
| | | | • | | | | | |

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| ATOM | 3169 | OH2 WAT | S 182 | 43.893. | 35.526 | 52:018 | 1.00 47.3 | 14 8 |
|--------------|--------------|---------|---------|------------------|------------------|------------------|-----------|------|
| ATOM | 3170 | OH2 WAT | S 183 | 29.166 | 21.424 | 28.950 | 1.00 45.0 | 8 80 |
| ATOM | 3171 | OH2 WAT | S 184 | 51.175 | 51.545 | 62.599 | 1.00 33.8 | 38 8 |
| ATOM | 3172 | OH2 WAT | S 185 | 18.520 | 46.208 | 42.323 | 1.00 50.8 | 35 8 |
| MOTA | 3173 | OH2 WAT | S 186 | 44.774 | 30.219 | 38.653 | 1.00 45.3 | 36 8 |
| ATOM | 3174 | OH2 WAT | S 187 | 30.770 | 9.460 | 69.837 | 1.00 32.4 | 14 8 |
| MOTA | 3175 | OH2 WAT | S 188 | . 22.157 | 39.535 | 78.736 | 1.00 37.0 | 01 8 |
| ATOM | 3176 | OH2 WAT | ' S 189 | 11.778 | 50.526 | 68.987 | 1.00 41.3 | 34 8 |
| MOTA | 3177 | OH2 WAT | ' S 190 | 31.339 | 60.910 | 49.439 | 1.00 21.8 | 8 8 |
| ATOM | 3178 | OH2 WAT | ' S 191 | 31.165 | 14.244 | 74.907 | 1.00 27.4 | |
| ATOM | 3179 | OH2 WAT | S 192 | 39.705 | 15.398 | 70.464 | 1.00 47.0 | |
| ATOM | 3180 | OH2 WAT | S 193 | 3.668 | 34.304 | 72.937 | 1.00 39.8 | |
| ATOM | 3181 | OH2 WAT | S 194 | 25.256 | 9.360 | 67.925 | 1.00 33.2 | |
| MOTA | 3182 | OH2 WAT | S 195 | 47.575 | 17.667 | 48.773 | 1.00 40.7 | |
| MOTA | 3183 | OH2 WAT | | 32.017 | 13.045 | 34.633 | 1.00 37.0 | |
| MOTA | 3184 | OH2 WAT | | 35.476 | 7.006 | 64.436 | 1.00 49.5 | |
| ATOM | 3185 | OH2 WAT | | 12.180 | 16.270 | 56.288 | 1.00 47.2 | |
| ATOM | 3186 | OH2 WAT | | 37.133 | 21.226 | 75.963 | 1.00 38.5 | |
| MOTA | 3187 | OH2 WAT | | 40.268 | 15.712 | 48.199 | 1.00 39.2 | - |
| MOTA | 3188 | OH2 WAT | | 25.159 | 17.768 | 46.858 | 1.00 49.8 | |
| MOTA | 3189 | OH2 WAT | | 24.593 | 27.104 | 65.727 | 1.00 53.4 | |
| MOTA | 3190 | OH2 WAT | | 36.741 | 20.267 | 33.858 | 1.00 41.9 | |
| ATOM | 3191 | OH2 WAT | | 10.013 | 53.930 | 47.546 | 1.00 48.0 | |
| MOTA | 3192 | OH2 WAT | | 22.305 | 16.731 | 54.471 | 1.00 27.0 | |
| MOTA | 3193 | OH2 WAT | | 47.454 | 34.778 | 74.101 | 1.00 47.4 | |
| MOTA | 3194 | OH2 WAT | | 35.189 | 55.767 | 45.193 | 1.00 59.4 | |
| ATOM | 3195 | OH2 WAT | | 37.827 | 18.151 | 36.382 | 1.00 45.3 | |
| MOTA | 3196 | OH2 WAT | | 6.823 | 37.405 | 51.989 | 1.00 58.2 | |
| ATOM | 3197 | OH2 WAT | | 32.040 17.038 | 43.551 | 36.157 | 1.00 30.7 | |
| MOTA | 3198 | OH2 WAT | | | 52.360 | 63.283 | 1.00 34.0 | |
| ATOM | 3199 | OH2 WAT | | 30.001 23.045 | 18.471 | 49.568 | 1.00 33.9 | |
| MOTA | 3200 3201 | OH2 WAT | | 26.130 | 28.615 61.496 | 33.729 75.246 | 1.00 44.2 | |
| MOTA MOTA | 3201 | OH2 WAT | - | 33.881 | 32.473 | 46.604 | 1.00 39.3 | |
| ATOM | 3202 | OH2 WAT | | 23.887 | 45.987 | 44.362 | 1.00 36.5 | |
| MOTA | 3204 | OH2 WAT | | 6.925 | 42.281 | 65.917 | 1.00 34.2 | |
| ATOM | 3205 | OH2 WAT | | 32.823 | 8.977 | 59.213 | 1.00 27.0 | |
| END | 2203 | Onz WAI | J 210 | 22.023 | 9.511 | | 2.00 27.0 | |
| لالالت | | | | | | | | |

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| Figure | 18-1 |
|--------|------|
| Liguio | 10-1 |

| Figure 18-1 | | | | | | | | |
|--------------|----------|----------|--------|----------|------------------|----------------------------------|--------------------------|----|
| | | | | Residue | # X | Y Z | B Segment | ID |
| ATOM | 1 | | ALA P | | 46.725 | | 1.00 56.80 | |
| MOTA | 2 | С | ALA A | . 2 | 47.943 | | | |
| ATOM | 3 | 0 | ALA A | | 48.857 | 13.292 137.884 | 1.00 60.99 | |
| ATOM | 4 | N | ALA A | | 46.995 | 14.046 140.488 | 1.00 56.88 | |
| ATOM | 5 | CA | ALA A | | 46.801 | 13.697 139.052 | 1.00 59.41 | |
| ATOM- | 6 | N | LYS A | | 47.890 | 11.525 138.903 | 1.00 53.41 | |
| MOTA | 7 | CA | LYS A | | 48.937 | 10.591 138.492 | 1.00 53.61 | |
| ATOM | 8 | CB | LYS A | | 48.736 | 9.229 139.156 | | |
| ATOM | 9 | CG | LYS A | | 48.917 | 9.279 140.665 | 1.00 50.26 | |
| ATOM | 10 | CD | TAS Y | | 48.950 | 7.891 141.285 | 1.00 56.64 | |
| ATOM | 11 | CE | LYS A | | 49.160 | 7.964 142.796 | 1.00 57.18 | |
| ATOM | 12 | NZ | LYS A | | 50.423 | | 1.00 56.74 | |
| ATOM | 13 | C | LYS A | | 49.063 | 8.663 143.165 10.430 136.986 | 1.00 54.86 | |
| ATOM | 14 | ō | LYS A | | 48.088 | 10.430 136.986 | | |
| ATOM | 15 | N | VAL A | | 50.287 | 10.147 136.550 | 1.00 44.34 | |
| ATOM | 16 | CA | VAL A | | 50.609 | 9.985 135.142 | 1.00 46.01 | - |
| ATOM | 17 | CB | VAL A | | 51.901 | 10.755 134.809 | 1.00 42.48 | - |
| ATOM | 18 | | VAL A | | 52.179 | 10.713 134.809 | 1.00 43.42 | |
| ATOM | . 19 | | VAL A | | 51.773 | 12.186 135.310 | 1.00 39.20 | |
| MOTA | 20 | C | VAL A | | 50.787 | 8.510 134.806 | 1.00 39.34 1.00 38.41 | |
| ATOM | 21 | ō | VAL A | | 51.659 | 7.839 135.351 | | |
| ATOM | 22 | N | LYS A | 5 | 49.959 | 8.011 133.899 | 1.00 37.08 | |
| ATOM | 23 | CA | LYS A | | 50.016 | 6.610 133.515 | 1.00 37.79 | |
| ATOM | 24 | CB | LYS A | 5 | 48.700 | 5.915 133.887 | 1.00 38.17 1.00 38.40 | |
| MOTA | 25 | CG | LYS A | 5 | 48.411 | 5.803 135.385 | 1.00 38.40 | |
| MOTA | 26 | CD | LYS A | 5 | 49.384 | 4.855 136.070 | 1.00 42.84 | |
| ATOM | 27 | CE | LYS A | 5 | 49.017 | 4.632 137.534 | 1.00 45.97 | |
| ATOM | 28 | NZ | LYS A | 5 | 49.045 | 5.894 138.322 | 1.00 51.78 | |
| ATOM | 29 | C | LYS A | 5 | 50.275 | 6.392 132.030 | 1.00 38.31 | |
| ATOM | 30 | 0 | LYS A | 5 | 49.992 | 7.253 131.201 | 1.00 38.13 | |
| MOTA | 31 | N | LEU A | 6 | 50.817 | 5.220 131.717 | 1.00 35.05 | |
| ATOM | 32 | CA | LEU A | 6 | 51.082 | 4.818 130.346 | 1.00 31.46 | |
| ATOM | 33 | CB | LEU A | 6 | 52.582 | 4.592 130.133 | 1.00 28.46 | |
| ATOM | 34 | CG | LEU A | 6. | 53.094 | 4.256 128.720 | 1.00 30.91 | |
| ATOM | 35 | CD1 | | 6 | 52.618 | 2.884 128.295 | 1.00 33.05 | |
| ATOM | 36 | CD2 | | 6 | 52.630 | 5.312 127.744 | 1.00 21.96 | |
| MOTA | 37 | C | LEU A | 6 | 50.307 | 3.512 130.164 | 1.00 30.50 | |
| ATOM | 38 | 0 | LEU A | 6 | 50.453 | 2.581 130.955 | 1.00 32.82 | |
| ATOM | 39 | N | ILE A | 7 7 | 49.459 | 3.456 129.145 | 1.00 26.94 | |
| ATOM ATOM | 40 41 | CA CB | ILE A | 7 | 48.676 47.218 | 2.255 128.893 2.598 128.493 | 1.00 28.29 | |
| ATOM | 42 | CG2 | ILE A | 7 | 46.499 | 1.343 128.041 | 1.00 28.94 1.00 32.57 | |
| ATOM | 43 | CG1 | ILE A | 7 | 46.447 | 3.172 129.688 | 1.00 32.57 | |
| ATOM | 44 | | ILE A | 7 | 46.979 | 4.468 130.236 | 1.00 46.80 | |
| ATOM | 45 | C | ILE A | 7 | 49.341 | 1.470 127.770 | 1.00 31.09 | |
| ATOM | 46 | 0 | ILT A | 7 | 49.600 | 2.009 126.695 | 1.00 27.65 | |
| ATOM | 47 | N | GL:A | 8 | 49.638 | 0.201 128.029 | 1.00 27.30 | |
| MOTA | 48 | CA | GL'. A | 8 | 50.27 7 | -0.614 127.016 | 1.00 25.50 | |
| MOTA | 49 | С | GLY A | 8 | 50.578 | -2.024 127.480 | 1.00 30.66 | |
| ATOM | 50 | 0 | GLY A | 8 | 50.224 | -2.421 128.592 | 1.00 30.02 | |
| ATOM | 51 | N | THR A | 9 | 51.238 | -2.777 126.611 | 1.00 28.94 | |
| ATOM | 52 | CA | THE A | 9 | 51.614 | -4.156 126.877 | 1.00 33.63 | |
| ATOM. | 53 | CB | THR A | 9 | 50.393 | -5.083 126.857 | 1.00 36.19 | |
| MOTA | 54 | OG1 | THR A | 9 | 50.827 | -6.441 126.992 | 1.00 34.87 | |
| ATOM | 55 | | | 9 | 49.633 | -4.931 125.548 | 1.00 36.49 | |
| ATOM | 56 57 | С | THR A | 9 | 52.567 | -4.637 125.794 | 1.00 34.83 | |
| ATOM | 57 50 | 0 | THE A | 9 | 52.545 | -4.133 124.677 -5.609 126.129 | 1.00 36.91 | |
| ATOM ATOM | 58 59 | N CA | LEU A | 10 10 | 53.407 54.345 | -5.609 126.129 -6.167 125.164 | 1.00 39.15 | |
| ATOM | 60 | CB | LEU A | 10 | 55.402 | -7.009 125.881 | 1.00 40.21 1:00 42.40 | |
| ATOM | 61 | CG | LEU A | 10 | 56.482 | -6.282 126.687 | 1.00 42.40 | |
| ATOM | 62 | | LEU A | 10 | 55.870 | -5.293 127.647 | 1.00 42.29 | |
| ATCM | 63 | | LEU A | 10 | 57.319 | -7.306 127.424 | 1.00 40.29 | |
| ATOM | 64 | C | LEU A | 10 | 53.591 | -7.039 124.159 | 1.00 41.70 | |
| ATOM | 65 | ō | LEU A | 10 | 54.055 | -7.266 123.044 | 1.00 37.13 | |
| ATOM | 66 | N | ASP A | 11 | 52.419 | -7.519 124.557 | 1.00 47.28 | |

| MOTA | 67 | CA | ASP A | 11 | 51.617 | -8.369 | | 1.00 53.30 |
|--------------|------------|----------|-------|------|------------------|-----------|--------------------|--------------------------|
| ATOM | 68 | CB | ASP A | | 50.230 | | 124.287 | 1.00 52.35 1.00 53.33 |
| MOTA | 69 | CG | ASP A | 11 | 50.295 | | 125.610 | 1.00 53.33 |
| ATOM | 70 | OD1 | ASP A | 11 | 51.004 | -10.358 | 125.685 | 1.00 52.21 |
| ATOM | 71 | OD2 | ASP A | . 11 | 49.630 | -8.883 | 126.567 | 1.00 53.33 |
| ATOM | 72 | С | ASP A | . 11 | 51.459 | | 122.257 | 1.00 54.31 |
| ATOM | 73 | 0 | ASP A | . 11 | 51.360 | | 121.311 | 1.00 54.31 |
| ATOM | 74 | N | TYR A | 12 | 51.424 | | 122.092 | 1.00 51.92 |
| ATOM | 75 | CA | TYR A | . 12 | 51.275 | -5.970 | 120.749 | 1.00 31.41 |
| MOTA | 76 | CB | TYR A | . 12 | 51.328 | -4.437 | 120.755 | 1.00 45.48 |
| ATOM | 77 | CG | TYR A | | 50.164 | -3.729 | 121.421 | 1.00 47.08 |
| ATOM | 78 | CD1 | TYR A | | 50.296 | -3.157 | | 1.00 47.53 |
| ATOM | 79 | CE1 | TYR A | | 49.252 | | 123.263 120.749 | 1.00 43.77 |
| ATOM | 80 | CD2 | TYR A | | 48.952 | | 120.749 | 1.00 44.16 |
| ATOM | 81 | CE2 | TYR A | _ | 47.906 | | 122.566 | 1.00 48.67 |
| ATOM | 82 | CZ | TYR A | | 48.061 | - | 123.116 | 1.00 48.65 |
| MOTA | 83 | OH | TYR A | | 47.030 52.367 | | 119.816 | 1.00 50.01 |
| ATOM | 84 | С | TYR A | | 52.367 | | 118.596 | 1.00 45.56 |
| ATOM | 85 | 0 | TYR A | | 53.484 | | | 1.00 48.72 |
| ATOM | 86 | N | GLY A | _ | 54.574 | | | 1.00 50.56 |
| MOTA | 87 | CA | GLY A | | 54.196 | | | 1.00 53.32 |
| ATOM | 88 | С | GLY A | | 54.931 | | | 1.00 52.64 |
| ATOM | 89 | 0 | GLY A | | 53.045 | | _ | 1.00 53.37 |
| MOTA | 90 | N | LYS A | | 52.55 | | | 1.00 54.56 |
| MOTA | 91 | CA | LYS A | | 52.022 | | | 1.00 58.02 |
| MOTA | 92 | CB | LYS A | | 53.086 | -12.062 | 120.591 | 1.00 62.81 |
| MOTA | 93 | CG | LYS A | | 53.934 | | 119.918 | 1.00 61.61 |
| MOTA | 94 95 | CD | LYS | | 54.74 | | | 1.00 61.77 |
| ATOM | 96 | NZ | LYS | | 55.514 | 1 -13.713 | | 1.00 58.35 |
| ATOM | 97 | C | LYS | | 51.45 | 5 -10.231 | | 1.00 52.03 |
| MOTA | 98 | Ö | LYS | | 50.91 | 1 -11.145 | 116.942 | 1.00 51.71 |
| MOTA MOTA | 99 | N | TYR | A 15 | 51.14 | | 117.372 | 1.00 46.92 |
| ATOM | 100 | CA | TYR | | 50.09 | | 116.449 | 1.00 47.99 |
| MOTA | 101 | CB | TYR | _ | 48.95 | | | 1.00 50.40 1.00 53.01 |
| ATOM | 102 | ĊG | TYR | A 15 | 48.45 | 6 -8.793 | | 1.00 52.10 |
| ATOM | 103 | CD1 | TYR | | 48.16 | | 119.637 | 1.00 51.72 |
| ATOM | 104 | CE: | L TYR | | 47.72 | | | 1.00 54.67 |
| ATOM | 105 | CD | 2 TYR | | 48.28 | | | 1.00 55.69 |
| ATOM | 106 | CE: | | | 47.83 | | | 1.00 54.18 |
| MOTA | 107 | CZ | TYR | | 47.56 47.13 | | - | 1.00 55.42 |
| MOTA | 108 | OH | TYR | | 50.59 | | | 1.00 46.20 |
| ATOM | 109 | C | TYR | | 49.93 | | | 1.00 43.72 |
| MOTA | 110 | 0 | TYR | | 51.75 | - | | 1.00 46.29 |
| ATOM | 111 | N | ARG | | 52.34 | 7 -7.10 | 9 113.727 | 1.00 45.66 |
| ATOM | 112 | CA | | | 53.77 | | 5 113.441 | 1.00 50.56 |
| ATOM | 113 | CB | | | 54.67 | 7 -7.69 | B 114.636 | 1.00 56.90 |
| ATOM | 114 | CG | | _ | 54.99 | 2 -6.38 | 8 115.315 | 1.00 60.72 |
| ATOM | 115 | CD NE | | | 56.02 | | 2 116.328 | 1.00 66.70 |
| ATOM | 116 117 | CZ | | | 57.21 | 1 -7.14 | 1 116.070 | |
| ATOM | 118 | NH | | _ | 57.52 | 0 -7.51 | 9 114.834 | 1.00 65.68 |
| MOTA | 119 | | 2 ARG | | 58.09 | 3 -7.31 | 4 117.046 | 1.00 66.33 |
| ATOM | 120 | | ARG | | 51.57 | 3 -7.29 | 8 112.429 | 1.00 44.20 |
| MOTA | 121 | | ARG | | 50.87 | | 3 112.254 | 1.00 43.41 |
| MOTA | 122 | | TYR | | 51.71 | | 6 111.514 | |
| MOTA MOTA | 123 | | | _ | 51.06 | | | |
| | 124 | | | _ | 50.91 | | | |
| atom atom | 125 | | | | 49.74 | 4 -4.25 | 5 110.084 | |
| ATOM | 126 | | | A 17 | 49.59 | 8 -3.98 | 2 111.443 | |
| atom | 127 | | | | 48.54 | | 4 111.909 | |
| ATOM | 128 | | | A 17 | 48.80 | | 0 109.204 | |
| ATOM | 129 | | | A 17 | 47.7 | | 5 109.656 | |
| ATOM | 130 | | TYR | A 17 | 47.6 | | 9 111.009 | |
| MOTA | 131 | | | | 46.6 | | 2 111.45 | |
| ATOM | 132 | | TYR | A 17 | 51.9 | 12 -1.35 | 0 109.36 | |
| | | | | | | | | |

```
53.150 -7.525 109.683
                                                           1.00 35.63
                         17
                  TYR A
        133
MOTA
                                         -7.925 108.278
                                                           1.00 46.68
                                  51.440
                         18
                  PRO A
ATOM
        134
             N
                                                            1.00 47.16
                                          -7.765 107.755
                                  50.076
                  PRO A
                         18
             CD
        135
                                                            1.00 48.87
MOTA
                                          -8.812 107.392
                                  52.205
                         18
                  ·PRO A
        136
              CA
MOTA
                                          -9.091 106.262
                                                           1.00 48.14
                                  51.213
                  PRO A
                         18
        137
              CB
MOTA
                                          -7.837 106.274
                                                            1.00 55.13
                                  50.343
                         18
                  PRO A
MOTA
        138
              CG
                                                            1.00 49.67
                                          -8.303 106.885
                                  53.556
                  PRO A
                         18
              С
        139
MOTA
                                                            1.00 49.33
                                          -7.101 106.766
                                  53.788
                         18
                  PRO A
        140
              0
                                                            1.00 53.22
MOTA
                                          -9.261 106.592
                                  54.432
                  LYS A
                         19
        141
              N
                                                            1.00 57.00
ATOM
                                          -9.044 106.114
                                  55.800
              CA
                  LYS A
                         19
        142
                                                            1.00 62.34
ATOM
                                  56.223 -10.242 105.252
                         19
                  LYS A
        143
              CB
MOTA
                                                            1.00 67.94
                                  55.069 -10.929 104.537
                  LYS A
                         19
        144
              CG
ATOM
                                                            1.00 70.76
                                         -9.963 103.714
                                  54.239
                  LYS A
                         19
         145
              CD
                                                            1.00 73.70
ATOM
                                  53.004 -10.653 103.162
                          19
              CE
                  LYS A
         146
ATOM
                                  52.116 --9.701 102.442
                                                            1.00 79.01
                  LYS A
                          19
         147
              ΝZ
                                         -7.757 105.405
-7.150 105.796
MOTA
                                                            1.00 55.93
                                  56.229
                  LYS A
                          19
         148
              С
                                                            1.00 59.86
MOTA
                                  57.230
                          19
                  LYS A
         149
              0
                                                            1.00 49.62
ATOM
                                           -7.338 104.367
                                  55.515
                          20
                  ASN A
MOTA
         150
              N
                                                            1.00 50.02
                                           -6.130 103.652
                                  55.925
                  ASN A
                          20
              CA
         151
MOTA
                                                            1.00 50.62
                                           -6.359 102.143
                                  55.829
                          20
                  ASN A
         152
              CB
ATOM
                                                            1.00 51.26
                                           -7.487 101.670
                                  56.729
                  ASN A
                          20
              CG
         153
ATOM
                                           -7.437 101.843
                                                            1.00 46.88
                                  57.948
                          20
         154
              OD1 ASN A
                                                            1.00 50.85
MOTA
                                           -8.513 101.074
                                  56.130
                          20
              ND2 ASN A
         155
MOTA
                                                            1.00 45.50
                                           -4.862 104.023
                                  55.167
                          20
                   ASN A
         156
              С
MOTA
                                                            1.00 45.35
                                           -3.778 103.533
                                  55.481
                          20
                   ASN A
         157
              0
                                                            1.00 37.46
MOTA
                                           -4.997 104.899
                                  54.182
                   HIS A
                          21
         158
              N
 MOTA
                                           -3.863 105.321
                                                            1.00 32.39
                                  53.374
                          21
                  HIS A
         159
              CA
                                                            1.00 29.34
 ATCM
                                           -4.355 106.162
                                   52.198
                   HIS A
                          21
              CB
         160
                                                            1.00 30.50
 ATCM
                                           -3.339 106.348
                                   51.118
                          21
              CG
                   HIS A
         161
 ATOM
                                           -2.314 107.223
                                                            1.00 22.88
                                   50.999
              CD2 HIS A
                          21
 MOTA
         162
                                                            1.00 30.15
                                           -3.298 105.552
                                   49.993
              ND1 HIS A
                          21
         163
 MOTA
                                                            1.00 30.96
                                           -2.293 105.933
                                   49.226
              CE1 HIS A
                          21
         164
                                                            1.00 36.41
                                           -1.680 106.945
 MOTA
                                   49.814
              NE2 HIS A
                          21
         165
                                                            1.00 29.18
 MOTA
                                           -2:879 106.155
                                   54.194
                          21
                   HIS A
         166
               C
 ATOM
                                           -3.279 106.963
                                                            1.00 26.92
                                   55.030
                   HIS A
                          21
         167
               0
 MOTA
                                           -1.572 105.969
                                                            1.00 31.12
                                   53.965
                          22
                   PRO A
         168
              И
 MOTA
                                                            1.00 29.46
                                           -0.912 105.043
                                   53.027
                   PRO A
                          22
               CD
         169
                                           -0.567 106.739
 ATOM
                                                             1.00 29.27
                                   54.702
                          22
         170
               CA
                   PRO A
                                                             1.00 26.00
 ATCM
                                            0.732 106.326
                                   54.012
                          22
                   PRO A
         171
               CB
 MOTA
                                                             1.00 31.52
                                            0.434 104.875
                                   53.670
                   PRO A
                          22
         172
               CG
                                                             1.00 29.96
 ATOM
                                            -0.822 108.253
                                   54.624
                   PRO A 22
          173
               С
                                                             1.00 27.47
 ATOM
                                           -0.538 108.981
                                   55.575
                   PRO A 22
          174
               0
 ATOM
                                                             1.00 26.64
                                            -1.371 108.715
                                   53.501
                           23
                   LEU A
          175
               N
                                                             1.00 30.44
 ATOM
                                            -1.644 110.144
                                   53.309
                           23
                   LEU A
               CA
          176
                                                             1.00 24.09
 ATOM
                                            -1.428 110.515
                                   51.833
                          23
          177
               CB
                   LEU A
                                                             1.00 25.30
 ATOM
                                             0.029 110.479
                                   51.356
                          23
                   LEU A
         . 178
               CG
 ATOM
                                                             1.00 17.72
                                             0.103 110.668
                                   49.836
               CD1 LEU A
                          23
          179
 ATCM
                                                             1.00 24.15
                                             0.816 111.574
                         23
                                   52.086
               CD2 LEU A
          180
 ATCM
                                                             1.00 31.64
                         23
                                          -3.015 110.662
                                   53.775
                   LEU A
          181
               С
                                                             1.00 31.00
 MOTA
                                            -3.512 111.667
                                   53.252
                   LEU A
                           23
          182
               0
                                                             1.00 28.25
 ATCM
                                            -3.636 110.012
                                   54.753
                           24
                   LYS A
          183
               N
  MOTA
                                                             1.00 30.90
                                            -4.929 110.513
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                           24
                   LYS A
                                                            1.00 36.59
          184
               CA
  ATOM
                                            -5.810 109.372
                                   55.718
                           24
                   LYS A
               CB
          185
  ATOM
                                                             1.00 40.77
                                            -5.650 108.982
                                   57.178
                   LYS A
                          24
          186
               CG
  MOTA
                                            -4.259 108.535
                                                             1.00 44.51
                                    57.546
                   LYS A
                           24
          187
               CD
                                                             1.00 50.44
  ATOM
                                            -4.303 107.755
                                    58.858
                           24
          188
                    LYS A
               CE
                                                             1.00 51.30
  ATOM
                                            -4.990 108.487
                                    59.959
                           24
          189
               NZ
                    LYS A
  ATCM
                                                              1.00 32.57
                                            -4.736 111.581
                                    56.282
                           24
                    LYS A
          190
               С
                                                              1.00 29.83
  ATOM
                                            -5.683 112.245
                                    56.695
                    LYS A
                           24
  ATOM
          191
               O
                                                              1.00 27.06
                                            -3.497 111.750
                                    56.729
                           25
          192
               N
                    ILE A
                                                              1.00 30.45
  ATOM
                                            -3.200 112.739
                                    57.755
                           25
                    ILE A
          193
               CA
                                                              1.00 33.37
  ATOM
                                            -1.822 112.499
                                    58.416
                           25
                    ILE A
                                                              1.00 33.22
          194
               CB
                                            -1.757 111.120
  ATOM
                                    59.056
               CG2 ILE A
                           25
          195
                                                              1.00 30.45
  ATCM
                                            -0.722 112.662
                                    57.361
                           25
               CG1 ILE A
          196
                                                              1.00 33.12
  ATCM
                                             0.689 112.700
                                    57.930
                CD1 ILE A
                           25
          197
                                                              1.00 32.10
 · ATCM
                                            -3.129 114.141
                                    57.156
                           25
                    ILE A
               С
  ATCM
          198
```

| | | | | | | 067 | -2.851 | 114.310 | 1.00 28.15 |
|------|-------|------|----------|------|---|--------|---------|---------------------|------------|
| ATOM | 199 | 0 | ILE A | 25 | | 55.967 | | | 1.00 31.64 |
| | 200 | N | PBO A | 26 | | 57.979 | | 115.168 | |
| ATOM | | | PRO A | 26 | | 59.395 | -3.768 | 115.139 | 1.00 31.11 |
| MOTA | 201 | CD | | | | 57.507 | -3.322 | 116.556 | 1.00 31.04 |
| ATOM | 202 | CA | PRO A | 26 | | | | 117.347 | 1.00 32.41 |
| ATOM | 203 | CB | PRO A | 26 | | 58.709 | | | |
| | 204 | CG | PRO A | 26 | | 59.454 | | 116.324 | |
| ATOM | | | PRO A | 26 | | 57.265 | -1.840 | 116.827 | 1.00 28.42 |
| MOTA | 205 | Ç. | | | | 58.001 | -0 994 | 116.315 | 1.00 22.23 |
| MOTA | 206 | 0 | PRO A | 26 | | | | 117.614 | 1.00 24.16 |
| MOTA | 207 | N | ARG A | 27 | | 56.251 | | | 1.00 28.53 |
| ATOM | 208 | CA | ARG A | 27 | | 55.977 | -0.116 | 117.899 | - |
| | | | ARG A | 27 | _ | 54.787 | 0.358 | 117.048 | 1.00 29.77 |
| MOTA | 209 | СВ | | | | 55.075 | | 115.554 | 1.00 29.64 |
| ATOM | 210 | CG | ARG A | 27 | | | | 114.620 | 1.00 26.61 |
| MOTA | 211 | CD | ARG A | 27 | | 53.918 | | | 1.00 28.52 |
| MOTA | 212 | NE | ARG A | 27 | | 53.622 | | 114.517 | 1.00 20.32 |
| | | CZ | ARG A | 27 | | 52.649 | 2.591 | 115.173 | 1.00 29.70 |
| MOTA | 213 | | | 27 | | 51.857 | 1.924 | 115.99 9 | 1.00 30.17 |
| ATOM | 214 | NH1 | | | | 52.451 | | 114.983 | 1.00 23.25 |
| MOTA | 215 | NH2 | ARG A | 27 | | | | 119.387 | 1.00 30.71 |
| ATOM | 216 | С | ARG A | 27 | | 55.746 | | | |
| | 217 | Ō | ARG A | 27 | | 56.679 | 0.490 | 120.113 | |
| MOTA | | | | 28 | | 54.529 | -0.117 | 119.863 | 1.00 23.51 |
| MOTA | 218 | 1,1 | VAL A | | | 54.282 | 0.093 | 121.282 | 1.00 29.33 |
| MOTA | 219 | CA | VAL A | 28 | | | | 121.635 | 1.00 34.56 |
| ATOM | 220 | CB | VAL A | 28 | | 52.800 | -0.124 | 121.033 | |
| | 221 | CG1 | | 28 | | 52.599 | | 123.142 | |
| ATOM | | | | 28 | | 51.947 | 0.908 | 120.903 | 1.00 33.77 |
| ATOM | 222 | CG2 | | | | 55.158 | -0.816 | 122.145 | 1.00 29.75 |
| ATOM | 223 | C | VAL À | 28 | | | | 123.182 | 1.00 32.49 |
| ATOM | 224 | 0 | VAL A | 28 | | 55.673 | | | 1.00 26.09 |
| ATOM | 225 | 20 | SER A | 29 | | 55.341 | -2.059 | 121.718 | |
| | | CA | SER A | 29 | | 56.162 | -2.982 | 122.483 | 1.00 31.39 |
| ATOM | 226 | | | 29 | | 56.058 | -4.399 | 121.905 | 1.00 26.92 |
| MOTA | 227 | CB | SER A | | | 56.562 | -4 464 | 120.579 | 1.00 33.85 |
| ATOM | 228 | oG | SER A | 29 | | | | | 1.00 34.77 |
| ATOM | 229 | С | SER A | 29 | • | 57.609 | -2.482 | | |
| | 230 | ō | SER A | 29 | | 58.378 | -2.718 | 123.391 | |
| ATOM | | | LEU A | 30 | | 57.967 | -1.778 | 121.380 | 1.00 31.20 |
| ATOM | 231 | :1 | | | | 59.317 | -1 -234 | 121.240 | 1.00 32.03 |
| ATOM | 232 | CA | LEU A | 30 | | | 0 660 | 119.829 | 1.00 30.86 |
| ATOM | 233 | CB | LEU A | 30 | | 59.554 | -0.000 | 110.020 | 1.00 33.22 |
| ATOM | 234 | CG | LEU A | 30 | | 61.008 | -0.550 | 119.333 | |
| | | נפס | | 30 | | 61.066 | 0.484 | 118.224 | 1.00 28.76 |
| MOTA | 235 | | | 30 | | 61.948 | -0.135 | 120.441 | 1.00 35.11 |
| MOTA | 236 | CD2 | | | | 59.423 | _0 089 | 122.236 | 1.00 30.29 |
| MOTA | 237 | С | LEU A | 30 | | | 0.005 | 122.984 | 1.00 27.69 |
| ATOM | 238 | Э | LEU À | 30 | | 60.397 | 0.019 | 122.904 | 1.00 27.38 |
| · · | 239 | M | LEU A | 31 | | 58.408 | | 122.232 | 1.00 27.30 |
| ATOM | | ĈΑ | LEU A | 31 | | 58.372 | 1.915 | | 1.00 24.94 |
| MOTA | 240 | | | 31 | | 57.008 | 2.596 | 123.042 | 1.00 24.92 |
| ATOM | 241 | CB | LEU A | | | 56.918 | 4.069 | | 1.00 30.49 |
| MOTA | 242 | CG | LEU A | 31 | | | | | 1.00 24.71 |
| MOTA | 243 | CD: | 1 LEU A | 31 | | 55.492 | 4.390 | | 1.00 27.32 |
| | 244 | CD. | 2 LEU A | 31 | | 57.851 | 4.355 | 124.603 | 1.00 27.32 |
| MOTA | | | | | | 58.610 | 1.429 | 124.564 | 1.00 28.18 |
| MOTA | 245 | C | LEU A | | | 59.489 | 1 928 | 125.263 | 1.00 33.64 |
| ATOM | 246 | ာ | LEU A | | | | 0.445 | 125.000 | 1.00 30.17 |
| MOTA | 247 | N | LEU A | | | 57.831 | 0.44 | . 122.000 | 1.00 30.59 |
| | 248 | CA | | | | 57.965 | -0.084 | 1 126.357 | 1.00 30.35 |
| MOTA | | | | | | 56.944 | -1.20 | 5 126.601 | 1.00 30.55 |
| ATOM | 249 | | | | | 55.458 | -0.879 | 126.402 | 1.00 29.50 |
| MOTA | 250 | | LEU A | | | 54.611 | _2 10 | 7 126.727 | |
| ATOM | 251 | CD | 1 LEU A | . 32 | | | -2.10 | 127 207 | |
| ATOM | . 252 | | 2 LEU A | 32 | | 55.058 | | 3 127.287 | |
| | | | LEU A | _ | | 59.376 | -0.59 | 7 126.657 | 1.00 33.56 |
| MOTA | 253 | | | | | 59.961 | | | 1.00 36.51 |
| MOTA | 254 | | LEU A | | | 59.926 | _ | | |
| ATOM | 255 | N | ARG A | | | | | | |
| | 256 | | | | | 61.271 | | | |
| ATOM | | | | | | 61.630 | -3.00 | | |
| ATOM | 257 | | | | | 60.814 | | 3 125.024 | |
| ATOM | 258 | | | | | | _ | | 1.00 53.68 |
| ATOM | 259 | CD | ARG A | 33 | | 61.237 | _ | | |
| | 260 | | | | | 60.515 | | 2 124.00/ | |
| MOTA | | | | | | 60.611 | _7.38 | 4 125.014 | |
| ATOM | 261 | | | | | 61.402 | | | 1.00 59.32 |
| ATOM | 262 | | 1 ARG | 33 | | 59.911 | | | 1.00 57.91 |
| ATOM | 263 | 3 NH | 12 ARG 2 | 33 | | | -0.31 | 5 125.978 | |
| | 264 | | ARG A | | | 62.314 | -0.84 | 5 143.5/6 | , 1.00 2 |
| ATOM | | | | | | | | | |

| | | | | | 6 | | | |
|--|--|--|---|---|---|--|---|--------------------------|
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 26567890123456789012322222222222222222222222222222222222 | COUCON CECCON CON CECCOOCON CECCON CECCON CON CECCON CEC | ASP A A A A A A A A A A A A A A A A A A | 334444444455555555566666666677777788888889999999999 | 883 63.10427 63.62.6173 64.8258 63.652.653.653.7416 63.652.653.653.7416 63.757.757.757.757.757.757.757.757.757.75 | 0.146 1.253 2.180 3.202 2.819 4.546 3.763 5.501 5.108 2.0294 2.432 3.5752 4.974 3.5752 4.974 3.827 2.387 2.387 2.387 2.387 2.387 0.127 0.187 0.1 | 122.783 126.305 126.852 126.802 128.042 128.374 127.395 127.790 127.688 128.548 129.183 130.043 129.190 130.242 130.126 131.157 132.360 130.765 130.174 131.201 128.958 128.768 129.244 129.714 129.545 131.502 131.502 131.657 133.039 134.050 132.188 132.170 130.812 | 1.00 40.42 |
| | | | | | 64.375 | 5.40 | 2 134.050 | 1.00 42.74 |
| | 315 | | LEU A | | | | 6 132.188 9 132.170 | |
| | | | | | | 6.61 | 0 130.812 | 1.00 40.42 |
| ATOM ATOM | 317 | | LEU A | | 63.940 | 7.07 | 4 130.447 | |
| ATOM · | | CD | 1 LEU A | 40 | 63.916 | | 3 129.088 1 131.513 | |
| MOTA | 320 | | 2 LEU A | | 64.470 60.967 | | 0 132.505 | 1.00 38.97 |
| ATOM | 321 | | LEU A | _ | 60.076 | 6.40 | 9 132.213 | 1.00 32.32 |
| ATOM ATOM | 322 323 | | ILE A | | 60.720 | 4.46 | 1 133.124 | 1.00 38.57 |
| ATOM | 324 | CA | ILE A | 41 | 59.363 | 3 4.10 5 3.57 | | 1.00 39.13 |
| ATOM | 325 | | | | 58.536 .59.137 | 7 2.27 | 11 131.820 | 1.00 36.51 |
| ATOM | 326 327 | | _ | | 57.082 | 2 3.36 | 57 132.774 | 1.00 38.71 |
| atom atom | 328 | | | 41 | 56.147 | 7 2.92 | 0 131.676 | 1.00 44.09 1.00 42.40 |
| ATOM | 329 | | ILE A | 41 | 59.376 | | 56 134.619 95 134.654 | |
| ATCM | 330 | 0 | ILE A | 41 | 60.25 | 2.13 | , LJE.UJ4 | |

| | | | | | | | 2 240 | 135.532 | 1.00 4 | 17 83 |
|------|------|------|---------|----|------|-------|---------|------------------------|--------|---------|
| ATOM | 331 | N | ASP A | 42 | 58.4 | | | | 1.00 | |
| ATOM | 332 | CA | ASP A | 42 | 58.3 | 01 | | 136.620 | | |
| ATOM | 333 | CB | ASP A | 42 | 58.2 | 43 | 2.880 | 137.984 | 1.00 | |
| | | CG | ASP A | 42 | 59.4 | | 3.688 | 138.284 | | 52.63 |
| MOTA | 334 | | | 42 | 60.6 | | 3.146 | 138.141 | 1.00 | 49.28 |
| MOTA | 335 | | ASP A | | 59.3 | | | 138.678 | 1.00 | 52.47 |
| ATOM | 336 | OD2 | ASP A | 42 | | | | 136.405 | 1.00 | |
| ATOM | 337 | С | ASP A | 42 | 57.0 | | | | 1.00 | |
| ATOM | 338 | 0 | ASP A | 42 | 56.0 | | | 135.864 | | |
| | 339 | N | GLU A | 43 | 57.0 | | | 136.832 | 1.00 | 21.41 |
| ATOM | | CA | GLU A | 43 | 55.9 | | | 136.673 | | 50.67 |
| ATOM | 340 | | | 43 | 56.2 | 34 - | -2.094 | 137.412 | 1.00 | |
| ATOM | 341 | CB | GLU A | | 55.2 | | | 137.185 | 1.00 | 60.55 |
| MOTA | 342 | CG | GLU A | 43 | | | -4.432 | 137.974 | | 66.12 |
| ATOM | 343 | CD | GLU A | 43 | 55.5 | | | 137.861 | | 70.33 |
| MOTA | 344 | OE1 | GLU A | 43 | 54.7 | | -5.417 | | 1.00 | |
| ATOM | 345 | | GLU A | 43 | 56.5 | | -4.427 | 138.711 | 1.00 | 50.33 |
| | 346 | C | GLU A | 43 | 54.6 | 45 - | -0.178 | 137.178 | | 50.20 |
| MOTA | | 0 | GLU A | 43 | 53.5 | 67 | -0.475 | 136.658 | | 48.27 |
| ATOM | 347 | | | 44 | 54.7 | | 0.683 | 138.186 | 1.00 | 49.04 |
| MOTA | 348 | N | LYS A | | 53.6 | | | 138.778 | 1.00 | 47.56 |
| ATOM | 349 | CA | LYS A | 44 | 54.0 | | 2.004 | 140.112 | | 54.73 |
| ATOM | 350 | CB | LYS A | 44 | | | | 140.542 | | 58.07 |
| MOTA | 351 | CG | LYS A | 44 | 53.1 | | 3.229 | | | 61.24 |
| ATOM | 352 | CD | LYS A | 44 | 53.7 | | | 139.853 | | |
| | 353 | CE | LYS A | 44 | 52.8 | 349 | 5.727 | 140.151 | | 61.93 |
| MOTA | | NZ | LYS A | 44 | 51.9 | 501 | 5.644 | 139.519 | | 62.80 |
| MOTA | 354 | | LYS A | 44 | 52.9 | | 2.387 | 137.875 | 1.00 | 44.52 |
| MOTA | 355 | С | | | 51. | | 2.701 | | 1.00 | 45.31 |
| MOTA | 356 | 0 | LYS A | 44 | 53.0 | | 2.915 | 136.914 | 1.00 | 41.03 |
| ATOM | 357 | N | GLU A | 45 | | | 3.914 | 135.994 | 1 00 | 41.23 |
| ATOM | 358 | CA | GLU A | 45 | 53. | | | | 1 00 | 38.52 |
| ATOM | 359 | CB | GLU A | 45 | 54.3 | | 4.810 | | | 40.30 |
| ATOM | 360 | CG | GLU A | 45 | 54.5 | 973 | 5.572 | | | |
| | 361 | CD | GLU A | 45 | 56.3 | 241 | 6.222 | | | 38.06 |
| ATOM | | | | 45 | 57. | 170 | 5.478 | 135.715 | 1.00 | 36.93 |
| MOTA | 362 | OE1 | | 45 | 56. | | 7.467 | 136.084 | 1.00 | 32.57 |
| ATOM | 363 | QE2 | | | 52. | | 3 : 253 | | 1.00 | 40.69 |
| MOTA | 364 | С | GLU A | 45 | | | 3.907 | | | 39.77 |
| ATOM | 365 | 0 | GLU A | 45 | 51. | | | | | 36.90 |
| ATOM | 366 | N | LEU A | 46 | 52. | | 1.953 | | 1.00 | 40.46 |
| ATOM | 367 | CA | LEU A | 46 | 52. | | 1.207 | | | |
| ATOM | 368 | CB | LEU A | 46 | 53. | 222 | 0.219 | | | 35.52 |
| | 369 | CG | LEU A | 46 | 52. | 873 | -0.619 | | 1.00 | 43.75 |
| MOTA | | | | 46 | 52. | 571 | 0.292 | | 1.00 | 42.06 |
| MOTA | 370 | CDI | - | 46 | | 035 | -1.544 | 131.500 | 1.00 | 42.90 |
| ATOM | 371 | CD2 | | | | 852 | 0.467 | | 1.00 | 40.03 |
| MOTA | 372 | С | LEU A | 46 | | | -0.306 | | 1.00 | 39.37 |
| ATOM | 373 | 0 | LEU A | 46 | | 741 | | | 1 00 | 34.03 |
| MOTA | 374 | N | ILE A | 47 | | 861 | 0.718 | | 1.00 | |
| MOTA | 375 | CA | ILE A | 47 | | 560 | 0.068 | - - | | 32.35 |
| TOM | 376 | | TLE A | 47 | | 413 | 1.087 | 132.937 | | |
| | 377 | ce' | 2 ILE A | 47 | 46. | 069 | 0.360 | 132.833 | 1.00 | 30.60 |
| MOTA | | | | _ | | 448 | 2.015 | 3 134.156 | 1.00 | 36.56 |
| LOW | 378 | CG: | | | | 372 | 3.080 | 134.162 | 1.00 | 35.46 |
| ATOM | 379 | CD: | | | | 428 | -0 920 | 131.882 | 1.00 | 33.67 |
| MOTA | 380 | C | ILE A | | | | -0.532 | 130.717 | | 27.64 |
| ATOM | 381 | 0 | ILE A | | | 505 | -0.332 | | 1 00 | 32.98 |
| MOTA | 382 | N | LYS A | 48 | | .231 | -2.19 | | | 30.98 |
| MOTA | 383 | CA | | | 48. | .102 | -3.224 | | | 30.30 |
| | 384 | CB | LYS A | _ | 48. | .038 | -4.609 | 9 131.821 | | 39.21 |
| MOTA | | | LYS A | | 47. | .956 | -5.74° | 7 130.819 | 1.00 | 46.81 |
| MOTA | 385 | CG | | _ | | . 989 | -7.10 | | 1.00 | 50.75 |
| ATOM | 386 | | | | | .967 | -8.24 | | 1.00 | 54.43 |
| ATOM | 387 | CE | | | | | -8.19 | | | 50.43 |
| ATOM | 388 | | LYS A | | | .151 | -0.19 | 2 129.300 2 120 210 | | 29.55 |
| | 389 | | LYS A | | | .869 | | 6 130.310 | | 29.65 |
| ATOM | 390 | | LYS A | | 45 | .764 | -2.84 | | | , 23.03 |
| ATOM | | | SER A | | | .071 | -2.99 | | | 30.69 |
| ATOM | 391 | | | | | .989 | -2.80 | 2 128.033 | | 29.32 |
| ATOM | 392 | | | | 46 | .551 | -2.80 | | 1.00 | 31.53 |
| ATOM | 393 | CB | SER A | | | | -1.83 | | 1.00 | 30.74 |
| ATOM | 394 | l OG | SER A | | | .571 | -1.01 | 6 128.147 | | 31.31 |
| ATOM | 395 | | SER A | | 44 | .952 | -3.91 | 0 120.14 | | 34.44 |
| | 396 | | SER A | | 45 | .295 | -5.05 | 9 128.436 | 1.0 | |
| atom | ,,,, | | - | | | | | | | |

| | | | | | _ | • | | | |
|--------------|------------|-----------|----------------|----------|---|------------------|------------------|-------------------------|--------------------------|
| MOTA | 397 | N | ARG A | 50 | | 43.688 | | 127.922 | 1.00 32.87 1.00 31.45 |
| ATOM | 398 | CA | ABG A | 50 | | 42.632 | | 127.960 129.101 | 1.00 31.45 |
| ATOM | 399 | CB | ARG A | 50 | | 41.636 | -4.325 -3.103 | 128.915 | 1.00 32.05 |
| ATOM | 400 | CG | ARG A | 50 | | 40.729 39.653 | -3.103 | 130.008 | 1.00 30.46 |
| MOTA | 401 | CD | ARG A | 50 | | 38.821 | -1.850 | 129.964 | 1.00 25.21 |
| MOTA | 402 | NE | ARG A | 50 50 | | 37.930 | -1.569 | 129.016 | 1.00 28.32 |
| ATOM | 403 | CZ NH1 | ARG A ARG A | 50 | | 37.726 | -2.406 | 128.001 | 1.00 25.45 |
| ATOM | 404 405 | NH2 | ARG A | 50 | | 37.238 | -0.439 | 129.087 | 1.00 24.92 |
| MOTA MOTA | 406 | C | ARG A | 50 | | 41.894 | | 126.638 | 1.00 31.12 1.00 24.62 |
| ATOM | 407 | ō | ARG A | 50 | | 41.895 | -3.406 | 126.019 126.181 | 1.00 24.02 |
| ATOM | 408 | N | PRO A | 51 | | 41.264 | -5.566 -6.921 | 126.751 | 1.00 32.40 |
| ATOM | 409 | CD | PRO A | 51 | | 41.164 40.534 | -5.506 | 124.917 | 1.00 30.36 |
| MOTA | 410 | CA | PRO A | 51 51 | | 40.138 | -6.967 | 124.683 | 1.00 33.95 |
| ATOM | 411 412 | CB CG | PRO A PRO A | 51 | | 41.173 | -7.750 | 125.499 | 1.00 32.85 |
| MOTA | 413 | C | PRO A | 51 | | 39.309 | | 125.134 | 1.00 31.61 1.00 29.84 |
| ATOM ATOM | 414 | Õ | PRO A | 51 | | 38.877 | -4.431 | 126.267 | 1.00 29.84 1.00 29.09 |
| ATOM | 415 | N | ALA A | 52 | | 38.755 | -4.093 -3.294 | 124.058 124.183 | 1.00 29.61 |
| ATOM | 416 | CA | ALA A | 52 | | 37.556 37.365 | -3.234 -2.447 | 122.956 | 1.00 28.67 |
| ATOM | 417 | CB | ALA A | 52 52 | | 36.437 | -4.321 | | 1.00 32.39 |
| ATOM | 418 | C | ALA A ALA A | 52 52 | | 36.603 | -5.453 | 123.844 | 1.00 30.40 |
| MOTA | 419 420 | N O | THR A | 53 | | 35.318 | -3.947 | | 1.00 32.98 |
| MOTA | 421 | CA | THR A | 53 | | 34.192 | -4.868 | | 1.00 36.61 1.00 34.22 |
| MOTA MOTA | 422 | CB | THR A | 53 | | 33.253 | -4.514 | | 1.00 34.22 |
| ATOM | 423 | OG1 | | 53 | | 32:734 | -3.193 | 123.370 | 1.00 36.45 |
| ATOM | 424 | CG2 | | 53 | | 33.998 33.411 | -4.700 | 123.702 | 1.00 38.94 |
| MOTA | 425 | C | THR A | 53 53 | | 33.559 | -3.689 | 123.012 | 1.00 32.67 |
| ATOM | 426 427 | И | THR A LYS A | 54 | | 32.577 | -5.679 | 123.372 | 1.00 39.19 |
| MOTA | 428 | CA | LYS A | | | 31.792 | -5.595 | 122.152 | 1.00 40.71 1.00 41.68 |
| ATOM ATOM | 429 | CB | LYS A | | | 30.933 | -6.853 | 121.994 | 1.00 41.00 |
| ATOM | 430 | CG | LYS A | | | 30.367 | -7.034 | 120.508 | 1.00 51.82 |
| MOTA | 431 | CD | LYS A | | | 29.541 29.075 | -8.588 | 119.087 | 1.00 52.94 |
| MOTA | 432 | CE | LYS A | | | 30.216 | -8.879 | 118.182 | 1.00 54.26 |
| MOTA | 433 434 | NZ C | LYS A | | | 30.913 | -4.34 | 7 122.237 | 1.00 39.46 |
| MOTA MOTA | 435 | | LYS A | | | 30.719 | -3.63 | | 1.00 37.19 1.00 36.71 |
| MOTA | 436 | | GLU A | . 55 | | 30.404 | -4.07 | 5 123.434 3 123.665 | 1.00 36.18 |
| ATOM | 437 | | | | | 29.554 | -2.91 | 7 125.127 | 1.00 42.16 |
| MOTA | 438 | | | | | 29.109 28.223 | -1.69 | | 1.00 46.04 |
| ATOM | 439 | | | | | 27.873 | -1.63 | 9 126.953 | 1.00 51.15 |
| MOTA | 440 441 | CD | 1 GLU A | | | 27.092 | -0.74 | 8 127.343 | 1.00 56.53 |
| ATOM ATOM | 442 | | 2 GLU A | - | | 28.382 | -2.48 | 2 127.727 | 1.00 51.67 1.00 35.45 |
| ATOM | 443 | | GLU A | 55 | | 30.278 | | 7 123.32: 9 122.66 | 1.00 33.43 |
| ATCM | 444 | | GLU A | | | 29.721 31.518 | | 6 123.776 | |
| ATOM | 445 | | GLU A | | | 32.289 | | 9 123.497 | 1.00 34.70 |
| MOTA | 146 | | | | | 33.635 | -0.32 | 9 124.232 | 1.00 30.71 |
| ATOM | 447 | | | | | 33.474 | -0.48 | 4 125.746 | 1.00 35.09 |
| MOTA MOTA | 449 | | | | | 34.787 | | 5 126.479 | 1.00 32.29 |
| MOTA | 450 | | 1 GLU | | | 35.645 | | 4 125.986 | |
| MOTA | 45 | | E2 GLU | a 56 | | 34.951 | | 4 127.569 4 121.988 | |
| ATCM | 45 | | GLU 3 | | | 32.495 32.341 | | 0 121.444 | 1.00 29.59 |
| ATOM | 45 | | GLU A | | | 32.827 | | 6 121.311 | 1.00 35.58 |
| ATOM | 45 | | | | | 33.039 | -1.14 | 17 119.871 | 1.00 35.70 |
| ATCM | 45: | | | | | 33.475 | -2.51 | 12 119.334 | 1 1.00 35.25 |
| ATOM | 45 45 | | | | | 34.829 | -3.03 | 30 119.814 | 1.00 36.19 1.00 33.69 |
| ATOM ATOM | 45 | | D1 LEU | A 57 | | 35.095 | | 0 119.183 | |
| ATOM | 45 | | D2 LEU | A 57 | | 35.925 | | 11 119.431 17 119.15 | |
| ATOM | 46 | 0 C | | | | 31.772 31.828 | | 67 118.20 | 5 1.00 32.72 |
| ATOM | 46 | | | | | 30.63 | | 28 119.62 | |
| ATOM | 46 | 2 N | LEU | M 36 | | ,,,,,,, | | | |
| | | | | | | | | | |

| ATOM | 463 | CA LEU A | 58 | 29.353 28.260 | -0.898 119 -1.844 119 | | 1.00 33.21 1.00 35.17 |
|--------------|------------|---------------------------------------|----------|------------------|--------------------------|----------------|--------------------------|
| ATOM | 464 | CB LEU A | 58 58 | 28.504 | -3.296 119 | .077 | 1.00 33.71 |
| ATOM | 465 | CD1 LEU A | 58 | 27.338 | -4.166 119 | .524 | 1.00 36.80 |
| ATOM | 466 | CD2 LEU A | 58 | 28.665 | -3.364 117 | 7.570 | 1.00 36.50 |
| ATOM | 467 468 | C LEU A | 58 | 28.940 | 0.543 119 | 222 | 1.00 30.99 |
| MOTA | 469 | D LEU A | 58 | 27.915 | 0.985 118 | 3.700 | 1.00 35.50 |
| MOTK MOTA | 470 | H LEU A | 59 | 29.733 | 1.279 119 | 9.993 | 1.00 32.55 |
| ATOM | 471 | CA LEU A | 59 | 29.443 | 2.687 120 | 0.217 | 1.00 30.37 |
| ATOM | 472 | CB LEU A | 59 | 30.387 | 3.279 12 | 1.268 | 1.00 28.01 1.00 32.19 |
| ATOM | 473 | CG LEU A | 59 - | 30.174 | 2.828 12 | 2./16 | 1.00 32.19 1.00 24.85 |
| ATOM | 474 | CD1 LEU A | 59 | 31.248 | 3.427 123 3.263 123 | 3.604 | 1.00 25.65 |
| ATOM | 475 | CD2 LEU A | 59 | 28.785 | 3.263 12. | 9.192 | 1.00 31.26 |
| ATOM | 476 | C LEU A | 59 | 29.632 29.020 | 4.442 11 | 8 652 | 1.00 31.80 |
| ATOM | 477 | O LEU A | 59 | 30.482 | 2.850 11 | 8.026 | 1.00 29.79 |
| ATOM | 478 | N PHE A | 60 60 | 30.726 | 3.454 11 | 6.716 | 1.00 30.24 |
| ATOM | 479 | CA PHE A | 60 | 32.131 | 4.055 11 | 6.637 | 1.00 29.99 |
| MOTA | 480 481 | CB PHE A | 60 | 32.443 | | 5.299 | 1.00 28.88 |
| MOTA | 482 | CD1 PHE A | 60 | 31.706 | | 4.845 | 1.00 25.58 |
| MOTA MOTA | 483 | CD2 PHE A | 60 | 33.448 | | 4.479 | 1.00 24.00 |
| MOTA | 484 | CE1 PHE A | 60 | 31.959 | 6.351 11 | 3.592 | 1.00 26.12 1.00 25.98 |
| ATOM | 485 | CE2 PHE A | 60 | 33.709 | | 3.226 | 1.00 25.98 1.00 24.53 |
| ATOM | 486 | CZ PHE A | 60 | 32.963 | | 2.781 5.529 | 1.00 30.30 |
| MOTA | 487 | C PHE A | 60 | 30.536 29.810 | | 4.602 | 1.00 32.82 |
| MOTA | 488 | O PHE A | 60 | 31.195 | | 5.543 | 1.00 32.85 |
| MOTA | 489 | N HIS A | 61 61 | 31.075 | 0.418 11 | | 1.00 34.59 |
| MOTA | 490 | CA HIS A | 61 | 32.296 | -0.492 11 | 4.361 | 1.00 32.89 |
| MOTA | 491 492 | CB HIS A | 61 | 33.576 | 0.238 11 | 4.116 | 1.00 34.25 |
| ATOM | 493 | CD2 HIS A | 61 | 34.225 | 0.532 11 | | 1.00 34 67 |
| MOTA MOTA | 494 | ND1 HIS A | 61 | 34.328 | • • - | 15.133 | 1.00 37.78 1.00 37.50 |
| ATOM | 495 | CE1 HIS A | 61 | 35.390 | | 14.619 | 1.00 37.50 1.00 37.91 |
| ATOM | 496 | ME2 HIS A | 61 | 35.350 | 1.243 11 | L3.307 | 1.00 38.44 |
| ATOM | 497 | C HIS A | 61 | 29.824 29.213 | -0.449 12 | 15 538 | 1.00 35.78 |
| ATOM | 498 | O HIS A | 61 | 29.213 | -1.015 1 | 13.327 | 1.00 39.73 |
| MOTA | 499 | N THR A | 62 62 | 28.278 | -1.868 1 | 13.218 | 1.00 38.05 |
| ATOM | 500 | CA THR A | 62 | 27.682 | -1.825 13 | 11.804 | 1.00 37.22 |
| MOTA | 501 502 | OG1 THR A | 62 | 28.631 | -2.345 1 | 10.867 | 1.00 41.15 |
| MOTA MOTA | 503 | CG2 THR A | | 27.348 | -0.404 1 | 11.418 | 1.00 38.27 1.00 39.06 |
| ATOM | 504 | C THR A | | 28.598 | -3.317 1 | 13.551 | 1.00 39.32 |
| ATOM | 505 | | 62 | 29.731 | -3.768 1 | 13.392 | 1.00 40.92 |
| ATOM | 506 | | | 27.582 | -4.034 1 -5.441 1 | 14.393 | 1.00 40.68 |
| ATOM | 507 | | | 27.696 26.303 | -6.000 1 | 14.704 | 1.00 43.19 |
| ATOM | 508 | | | 26.269 | -7.451 1 | 15.171 | 1.00 46.90 |
| atom | 509 | | | 26.472 | -7.593 1 | 16.665 | 1.00 53.11 |
| ATOM | 510 | | | 26.601 | -8.739 1 | 17.152 | 1.00 52.78 |
| ATOM | 511 512 | | | 26.487 | -6.556 1 | 17.358 | 1.00 57.24 |
| ATOM ATOM | 513 | | | 28.320 | -6.263 1 | 13.268 | 1.00 36.19 1.00 29.70 |
| ATOM | 514 | | | 29.272 | -7.011 1 | 13.481 | |
| ATOM | 515 | N ASP A | 64 | 27.755 | -6.119 1 | 10 006 | |
| ATOM | 516 | CA ASP A | | 28.198 | -6.841 1 -6.382 1 | 10.600 | |
| ATOM | 517 | | | 27.363 | -4.872 1 | 09.582 | 1.00 53.38 |
| ATOM | 518 | _ | | 27.313 28.290 | | .09.089 | 1.00 52.15 |
| MOTA | 519 | | | 26.298 | | 10.018 | 1.00 53.97 |
| ATOM | 520 | | | 29.673 | -6.660 | 110.594 | 1.00 35.04 |
| ATOM | 523 | | | 30.379 | -7.625 | L10.303 | 1.00 33.60 |
| ATOM | 523 | | | 30.144 | -5.423 | 110.671 | 1.00 33.88 |
| ATOM | 523 524 | | | 31.554 | -5.153 | 110.419 | |
| ATOM | 521 | | | 31.793 | | | |
| atom atom | 52 | 6 CG TYR A | A 65 | 33.247 | | 110.219 | |
| ATOM | 52 | · · · · · · · · · · · · · · · · · · · | | 34.009 | | 100 024 | |
| ATOM | 52 | | | 35.352 | -5.411 | 103.04 | |
| 0 | | | | | | | |

| • | | | | | | | | |
|----------------|------------|---------|------------------|----------|------------------|----------|-----------|--------------------------|
| | 500 | CD2 | TYR A | 65 | 33.863 | -2.398 | 111.134 | 1.00 34.08 [.] |
| ATOM | 529 | CE2 | TYR A | 65 | 35.211 | -2.050 | 111.002 | 1.00 29.89 |
| ATOM | 530 | | TYR' A | 65 | 35.949 | -2.560 | 109.948 | 1.00 35.29 |
| ATOM | 531 | CZ | TYR A | 65 | 37,286 | -2.231 | 109.825 | 1.00 29.81 |
| MOTA | 532 | ОН | | 65 | 32.405 | -5.813 | 111.504 | 1.00 27.65 |
| MOTA | 533 | C | TYR A | 65 | 33.339 | -6.557 | 111.209 | 1.00 27.65 |
| MOTA | 534 | 0 | TYR A | 66 | 32.070 | -5.559 | 112.765 | 1.00 27.32 |
| ATOM | 535 | N | ILE A | | 32.822 | -6.153 | 113.858 | 1.00 25.82 |
| MOTA | 536 | CA | ILE A | 66 | 32.227 | -5.764 | 115.217 | 1.00 32.25 |
| MOTA | 537 | CB | ILE A | 66 | 33.029 | -6.403 | 116.338 | 1.00 28.85 |
| MOTA | 538 | | -ILE A | 66 | 32.226 | -4.242 | 115.364 | 1.00 31.48 |
| MOTA | 539 | | ILE A | 66 | 33.607 | -3.612 | 115.282 | 1.00 38.02 |
| MOTA | 540 | CD1 | | 66 | 32.836 | -7.677 | 113.736 | 1.00 31.21 |
| MOTA | 541 | C | ILE A | 66 | 33.891 | -8.305 | 113.844 | 1.00 30.25 |
| MOTA | 542 | 0 | ILE A | 66 | 31.672 | -8.279 | 113.507 | 1.00 33.28 |
| MOTA | 543 | И | ASN A | 67 | 31.627 | -9.731 | | 1.00 35.87 |
| MOTA | 544 | CA | ASN A | 67 | 30.190 | | 113.177 | 1.00 33.07 |
| ATOM | 545 | CB | ASN A | 67 | 29.338 | -10.072 | | 1.00 37.34 |
| ATOM | 546 | CG | ASN A | 67 | 29.330 | -10.296 | | 1.00 35.20 |
| ATOM | 547 | OD1 | | 67 | 28.071 | -9.709 | | 1.00 34.83 |
| ATOM | 548 | ND2 | | 67 67 | 32.499 | | | 1.00 31.00 |
| MOTA | 549 | C | ASN A | 67 | 33.132 | -11.248 | | 1.00 37.26 |
| MOTA | 550 | 0 | ASN A | 67 68 | 32.543 | -9.426 | | 1.00 30.91 |
| MOTA | 551 | N | THR A | 68 | 33.368 | -9.814 | | 1.00 31.04 |
| MOTA | 552 | CA | THR A | 68 68 | 33.133 | -8.894 | | 1.00 34.01 |
| MOTA | 553 | CB | THR A | 68 | 31.780 | -9.037 | | 1.00 33.26 |
| MOTA | 554 | OG1 | | 68 | 34.072 | -9.256 | _ | 1.00 30.84 |
| ATOM | 555 | CG2 | THR A | 68 | 34.844 | -9.794 | | 1.00 33.31 |
| MOTA | 556 | С 0 | THR A | 68 | 35.591 | -10.708 | 110.024 | 1.00 32.52 |
| ATOM | 557 558 | N | LEU A | 69 | 35.267 | -8.768 | 111.117 | 1.00 30.30 |
| MOTA | 559 | CA | LEU A | 69 | 36.669 | -8.686 | 111.534 | 1.00 28.20 |
| MOTA | 560 | CB | LEU A | 69 | 36.938 | -7.409 | 112.351 | 1.00 28.25 |
| ATOM ATOM | 561 | CG | LEU A | 69 | 36.859 | -6.049 | | 1.00 30.18 |
| ATOM | 562 | CD1 | _ | 69 | 37.154 | -4.929 | | 1.00 31.08 |
| ATOM | 563 | | LEU A | 69 | 37.868 | ÷6.004 | | 1.00 27.85 |
| MOTA | 564 | C | LEU A | 69 | 37.036 | -9.902 | | 1.00 31.65 1.00 23.95 |
| MOTA | 565 | o | LEU A | 69 | 38.084 | -10.519 | | 1.00 23.93 |
| MOTA | 566 | N | MET A | 70 | 36.169 | -10.243 | | 1.00 34.50 |
| ATOM | 567 | CA | MET A | 70 | 36.411 | | | 1.00 31.96 |
| ATOM | 568 | CB | MET A | 70 | 35.318 | | | 1.00 36.26 |
| ATOM | 569 | CG | MET A | 70 | 35.203 | | | 1.00 37.52 |
| ATOM | 570 | SD | MET A | 70 | 33.948 | | 5 118.403 | 1.00 37.36 |
| MOTA | 571 | CE | MET A | 70 | 34.633 36.484 | | - | 1.00 33.33 |
| MOTA | 572 | С | MET A | 70 | 37.392 | | | 1.00 31.47 |
| MOTA | 573 | 0 | MET A | 70 | 35 534 | -12 88 | 7 112.494 | 1.00 35.37 |
| ATOM | 574 | N | GLU A | 71 | 35.534 | -14.09 | 8 111.681 | 1.00 36.6 |
| MOTA | 575 | CA | GLU A | 71 71 | 34 245 | -14.16 | 0 110.834 | 1.00 37.3 |
| MOTA | 576 | CB | GLU A | 71 | 34 206 | -15.35 | 9 109.897 | 1.00 46.37 |
| ATOM | 577 | CG | GLU A | 71 | 34 257 | -16.69 | 3 110.633 | 1.00 46.37 |
| atom | 578 | CD | | 71 | 34.355 | -17.73 | 3 109.952 | 1.00 48.94 |
| MOTA | 579 | | 1 GLU A | 71 | 34.190 | -16.70 | 5 111.882 | 1.00 45.53 |
| ATOM | 580 | OE. | 2 GLU A GLU A | | 36.732 | -14.16 | 9 110.769 | 1.00 35.96 |
| MOTA | 581 | C | GLU A | | 37.342 | -15.22 | 8 110.617 | 1.00 32.99 |
| ATOM | .582 | O N | ALA A | | 37.079 | -13.03 | 9 110.159 | 1.00 36.50 |
| MOTA | 583 | N C3 | | | 38.225 | -12.98 | 1 109.264 | 1.00 33.98 |
| MOTA | 584 585 | | | | 38.366 | 5 -11.58 | 0 108.675 | |
| MOTA | 585 | | ALA A | | 39.498 | 3 -13.36 | 2 109.998 | 1.00 34.60 |
| ATCM | 586 587 | | ALA A | | 40.337 | 7 -14.09 | 4 109.466 | |
| ATOM | 587 588 | | GLU A | | 39.647 | 7 -12.87 | 3 111.224 | 1.00 30.87 |
| ATOM | 589 | | | | 40.847 | 7 -13.17 | 7 111.985 | |
| ATOM | 590 | | | | 41.004 | 4 -12.22 | 4 113.180 | |
| ATOM | 591 | | _ | | 42.234 | 4 -12.54 | 5 114.033 | |
| ATOM | 592 | | | | 42 390 | 0 -11.63 | 4 115.233 | |
| ATOM · ATOM | 593 | OE | 1 GLU A | . 73 | 42.60 | 1 -10.41 | 8 115.044 | |
| ATOM | 594 | OE | 2 GLU A | 73 | 42.29 | 8 -12.13 | 8 116.372 | 1.00 41.21 |
| AION | | | | | | | | |

| | 505 | _ | GLU A | 73 | 40.906 | -14.615 | 112.485 | 1.00 31.73 |
|------|-----|-----|--------|------------|-----------|------------|------------|------------|
| ATOM | 595 | С | | | | | 112.409 | 1.00 32.96 |
| ATOM | 596 | 0 | GLU A | 73 | | -15.249 | | |
| | | | ARG A | 74 | 39.798 | -15.145 | 112.992 | 1.00 35.85 |
| MOTA | 597 | N | | | | | 113.502 | 1.00 43.24 |
| ATOM | 598 | CA | ARG A | 74 | 39.847 | -10.511 | | |
| | 599 | CB | ARG A | 74 | 38.548 | -16.892 | 114.216 | 1.00 43.63 |
| ATOM | | | | | | -17.349 | 113.294 | 1.00 51.20 |
| ATOM | 600 | CG | ARG A | 74 | | | | 1.00 51.13 |
| ATOM | 601 | CD | ARG A | 74 | | -18.087 | 114.063 | |
| | | | | | 25 53/ | -18.871 | 113.158 | 1.00 57.40 |
| ATOM | 602 | NE | ARG A | 74 | | | | 1.00 56.36 |
| ATOM | 603 | CZ | ARG A | . 74 | 35.99 | -19.870 | 112.403 | |
| | | | | 74 | 37.27 | -20.208 | 112.446 | 1.00 51.10 |
| MOTA | 604 | NH1 | | | | | | 1.00 58.75 |
| ATOM | 605 | NH2 | ARG A | 74 | | 2 -20.517 | | |
| | 606 | С | ARG A | 74 | 40.12 | 5 -17.506 | 112.372 | 1.00 43.06 |
| ATOM | | | | | | -18.429 | | 1.00 42.52 |
| MOTA | 607 | 0 | ARG A | 74 | | | | |
| | 608 | N | SER A | 75 | 39.48 | -17.305 | 111.222 | |
| MOTA | | | | 75 | 39.67 | -18.186 | 110.066 | 1.00 44.93 |
| MOTA | 609 | CA | SER A | | | | | 1.00 42.05 |
| ATOM | 610 | CB | SER A | 75 | 38.48 | 5 -18.089 | 109.113 | |
| | | | SER A | 75 | 38.42 | -16.799 | 108.532 | 1.00 38.43 |
| MOTA | 611 | og | | | 40.91 | | | 1.00 46.44 |
| MOTA | 612 | С | SER A | 75 | | | | |
| | 613 | 0 | SER A | 75 | 41.33 | 9 -18.522 | 108.383 | 1.00 45.17 |
| ATOM | | | | | 41.46 | 6 -16.638 | 109.618 | 1.00 46.18 |
| ATOM | 614 | N | GLN A | 76 | | | | 1.00 44.73 |
| ATOM | 615 | CA | GLN A | 76 | 42.64 | | | |
| | | CB | GLN A | 76 | 43.86 | B -16.973 | 109.226 | 1.00 37.36 |
| ATOM | 616 | | | | 45.16 | | | 1.00 43.96 |
| ATOM | 617 | CG | GLN A | 76 | | | | |
| | 618 | CD | GLN A | 76 | 45.41 | 5 -15.214 | 110.176 | 1.00 41.86 |
| MOTA | | | | | 44.49 | | 110.655 | 1.00 37.78 |
| ATOM | 619 | OE1 | GLN A | 76 | | | | 1.00 45.00 |
| MOTA | 620 | NE2 | GLN A | 76 | 46.66 | | 110.591 | |
| | | | GLN A | 76 | 42.37 | 4 -16.120 | 107.429 | 1.00 44.17 |
| MOTA | 621 | C | | | 43.23 | | 106.630 | 1.00 40.49 |
| MOTA | 622 | 0 | GLN A | 76 | | | | |
| | 623 | N | SER A | 77 | 41.16 | 8 -15.713 | 3 107.053 | |
| MOTA | | | | 77 | 40.78 | | 7 105.649 | 1.00 44.66 |
| ATOM | 624 | CA | SER A | | | | | 1.00 44.56 |
| ATOM | 625 | CB | SER A | 77 | 40.18 | | | |
| | | | SER A | 7 7 | 38.97 | 4 - 17.240 | 5 105.925 | 1.00 42.58 |
| MOTA | 626 | OG | | | 39.74 | | | 1.00 44.80 |
| ATOM | 627 | С | SER A | 77 | | | | |
| | 628 | 0 | SER A | 77 | 39.09 | 6 -14.142 | | |
| MOTA | | | | 78 | 39.59 | | 7 104.207 | 1.00 46.06 |
| ATOM | 629 | N | VAL A | | | | | 1.00 47.65 |
| ATOM | 630 | CA | VAL A | 78 | 38.63 | | | |
| | | | VAL A | 78 | 39.10 | 7 -12.24 | 5 102.701 | 1.00 49.63 |
| ATOM | 631 | CB | | | 38.07 | | 7 102.391 | 1.00 51.25 |
| ATOM | 632 | CG1 | VAL A | 78 | _ | | | 1.00 53.00 |
| MOTA | 633 | CG2 | VAL A | 78 | 40.45 | 4 -11.62 | 7 103.017 | |
| | | | | 78 | 37.27 | 5 -13.68 | 2 103.530 | 1.00 48.07 |
| MOTA | 634 | С | VAL A | | | | | 1.00 42.31 |
| MOTA | 635 | 0 | VAL A | 78 | 37.11 | | | |
| | 636 | N | PRO A | 79 | 36.28 | 2 - 13.49 | 2 104.407 | |
| ATOM | | | | 79 | 36.34 | | 2 105.696 | 1.00 50.81 |
| MOTA | 637 | CD | PRO A | | | | | 1.00 51.31 |
| ATOM | 638 | CA | PRO A | 79 | 34.92 | | | |
| | 639 | CB | PRO A | 79 | 34.17 | 0 -13.45 | 0 105.396 | 1.00 53.13 |
| MOTA | | | | -g | 35.24 | 4 -13.46 | 9 106.469 | 1.00 53.50 |
| ATOM | 640 | CG | PRO A | - | | | | 1.00 52.42 |
| MOTA | 641 | C | PRO A | ;9 | 34.34 | 3 -13.21 | 7 102.858 | 1.00 52.42 |
| | | | | . 9 | 34.67 | 0 -12.42 | 8 102.382 | 1.00 55.73 |
| ATOM | 642 | 0 | PRO A | | 22.40 | 2 -14.34 | 3 102.273 | 1.00 49.63 |
| ATOM | 643 | N | LYS A | 80 | 33.40 | 7 -14.34 | 2 102.273 | 1.00 51.62 |
| | 644 | CA | LYS A | 80 | 32.82 | 4 -14.05 | 3 101.002 | 1.00 51.02 |
| ATOM | | | | | 31 67 | 2 -15.00 | 4 100.822 | 1.00 53.92 |
| MOTA | 645 | CB | LYS A | 80 | 22.00 | 2 14 00 | 8 99.545 | 1.00 56.27 |
| MOTA | 646 | CG | LYS A | 80 | 30.81 | 7 -14.80 | 0 33.343 | |
| | | CD | LYS A | 80 | 29.58 | 36 -15.71 | 2 99.560 | 1.00 56.61 |
| MOTA | 647 | | | | 20 7/ | 4 -15.57 | 9 98.298 | 1.00 56.04 |
| MOTA | 648 | CE | LYS A | 80 | 20.7 | 14 -13.37 | | |
| | 649 | NZ | LYS A | 80 | 29.47 | 1 -16.03 | 6 97.081 | |
| MOTA | | | | | 20 Z | 8 -12.60 | 7 100.874 | 1.00 51.10 |
| ATOM | 650 | С | LYS A | 80 | . د . ع د | 10 10 14 | 0 101.689 | |
| ATOM | 651 | 0 | LYS A | 80 | 31.5 | 39 -12.14 | U TUI.007 | |
| | | | GLY A | | 32.83 | 21 -11.91 | .4 99.842 | |
| ATOM | 652 | N | | | 22 4 | 8 -10.53 | 7 99.592 | 1.00 47.07 |
| ATOM | 653 | CA | GLY A | | 22.4. | | | |
| | 654 | C | GLY A | | 32.8 | | | |
| ATOM | | | | | 32.6 | | 1 100.397 | 1.00 43.90 |
| ATOM | 655 | 0 | GLY A | | | | | |
| ATOM | 656 | N | ALA A | 82 | 33.5 | | | |
| | | | ALA A | | 33.9 | 73 -9.02 | 29 102.715 | 1,00 44.09 |
| ATOM | 657 | | י אייי | | 34.4 | | | 1.00 44.62 |
| ATOM | 658 | CB | ALA A | . 82 | | | | |
| ATOM | 659 | | ALA A | 82 | 35.0 | | | |
| | | | ALA A | | 35.1 | 32 -6.92 | 25 102.662 | 1.00 33.32 |
| ATOM | 660 | Ü | י אשה | | | | | |
| | | | | | | | | |

| | | | | | | | | | 1.00 43.30 |
|---------------|-----|------|-------|------|----------|--------|--------|-------------------|------------|
| ATOM | 661 | N | ARG A | 83 | | 35.874 | -8.549 | 101.289 | |
| | | | ARG A | | | 36.959 | -7.742 | 100.741 | 1.00 43.25 |
| MOTA | 662 | CA | | | | 37.715 | | 99.677 | 1.00 46.60 |
| MOTA | 663 | ÇВ | ARG A | | | | | | 1.00 51.32 |
| ATOM | 664 | CG | ARG A | 83 | | 38.988 | -7.865 | 99.222 | |
| | | | ARG A | | | 39.636 | -8.632 | 98.086 | 1.00 55.55 |
| MOTA | 665 | CD | | | | 40.995 | -8.164 | 97.810 | 1.00 64.08 |
| MOTA | 666 | NE | ARG A | | | | | - | 1.00 63.01 |
| ATOM | 667 | CZ | ARG A | 83 | | 41.330 | -6.905 | 97.540 | |
| | | NH1 | | | | 40.403 | -5.954 | 97.504 | 1.00 62.76 |
| MOTA | 668 | | | | | 42.599 | -6.600 | 97.304 | 1.00 59.66 |
| MOTA | 669 | NH2 | ARG A | | | | | 100.134 | 1.00 44.58 |
| ATOM | 670 | С | ARG A | ¥ 83 | | 36.453 | -6.435 | | 1.00 37.50 |
| | 671 | Ō | ARG A | | | 37.002 | -5.365 | 100.395 | 1.00 38.05 |
| MOTA | | | | | | 35.404 | -6.528 | 99.323 | 1.00 41.82 |
| ATOM | 672 | N | GLU A | | | | -5.356 | 98.678 | 1.00 41.44 |
| MOTA | 673 | CA | GLU A | A 84 | | 34.824 | | | 1.00 46.27 |
| | 674 | CB | GLU A | A 84 | | 34.145 | -5.765 | 97.367 | |
| MOTA | | ĊG | GLU Z | - | | 33.621 | -7.185 | 97.388 | 1.00 52.61 |
| MOTA | 675 | | | | | 34.749 | -8.198 | 97.308 | 1.00 54.12 |
| MOTA | 676 | CD | GLU A | | | | | 97.764 | 1.00 59.66 |
| ATOM | 677 | OE1 | GLU A | a 84 | 1 | 34.555 | -9.344 | | |
| | 678 | OE2 | | | | 35.823 | -7.850 | 96.769 | 1.00 50.30 |
| MOTA | | | | | | 33.831 | -4.595 | 99.545 | 1.00 37.36 |
| MOTA | 679 | С | GLU | | | | -3.379 | | 1.00 34.30 |
| ATOM | 680 | 0 | GLU A | | | 33.692 | | | 1.00 36.00 |
| ATOM | 681 | N | LYS | A 85 | , | 33.138 | | 100.427 | |
| | | CA | LYS | | | 32.154 | -4.646 | 101.280 | 1.00 36.95 |
| MOTA | 682 | | | | | 31.089 | -5.649 | 101.725 | 1.00 36.60 |
| ATOM | 683 | CB | LYS . | | | | -5.042 | | 1.00 40.72 |
| ATOM | 684 | CG | LYS . | A 85 |) | 29.975 | | | 1.00 46.21 |
| ATOM | 685 | CD | LYS . | A 85 | ; | 28.939 | -6.092 | | 1.00 40.41 |
| | | | LYS | | | 27.839 | -5.487 | 103.827 | 1.00 49.06 |
| MOTA | 686 | CE | | | | 26.859 | -6.513 | | 1.00 52.72 |
| ATOM | 687 | NZ | LYS | | | | | | 1.00 36.48 |
| ATOM | 688 | С | LYS | A 8! | 5 | 32.785 | -4.008 | 102.313 | |
| | 689 | ŏ | LYS | | 5 | 32.353 | -2.949 | | 1.00 32.97 |
| ATOM | | | | | | 33.819 | -4.649 | | 1.00 33.69 |
| MOTA | 690 | N | TYR | | | 34.468 | | 104.250 | 1.00 35.23 |
| ATOM | 691 | CA | TYR | | | | | | 1.00 33.65 |
| MOTA | 692 | CB | TYR | A 8 | 5 | 34.410 | -5.281 | | _ |
| | | CG | TYR | | | 32.990 | -5.665 | 105.680 | 1.00 35.09 |
| MOTA | 693 | | | | | 32.165 | -4.76 | | 1.00 34.06 |
| ATOM | 694 | CDI | | | | | -5.100 | | 1.00 34.32 |
| ATOM | 695 | CE | TYR | A 8 | 5 | 30.866 | | | 1.00 33.17 |
| | 696 | CD2 | TYR | A 8 | 6 | 32.470 | -6.923 | | |
| ATOM | | CE | | | | 31.162 | -7.27 | 105.716 | 1.00 33.91 |
| MOTA | 697 | | | | | 30.369 | -6.35 | | 1.00 34.21 |
| MOTA | 698 | CZ | TYR | | | | -6.65 | | 1.00 35.20 |
| ATOM | 699 | OH | TYR | A 8 | 6 | 29.079 | | | |
| | 700 | С | TYR | A 8 | 6 | 35.901 | -3.673 | | |
| MOTA | | | TYR | | | 36.552 | -3.20 | 3 104.984 | 1.00 36.06 |
| MOTA | 701 | 0 | | | | 36.382 | -3 77 | 7 102.814 | 1.00 36.46 |
| ATOM | 702 | N | ASN | | | | | | 1.00 32.71 |
| ATOM | 703 | CA | ASN | A 8 | 7 | 37.712 | -3.31 | | |
| | 704 | CB | ASN | | 7 | 37.768 | -1.79 | | |
| ATOM | | | ASN | | 7 | 38.989 | -1.19 | 9 101.926 | 1.00 37.25 |
| MOTA | 705 | CG | | | | 39.305 | -1.51 | | 1.00 36.29 |
| MOTA | 706 | OD: | | | 7 | | | | |
| ATOM | 707 | ND | 2 ASN | A 8 | 7 | 39.675 | -0.32 | 0 102.640 | 1.00 34.73 |
| | 708 | С | ASN | | 7 | 38.855 | | 6 103.217 | 1.00 34.73 |
| MOTA | | | | _ | 7 | 39.868 | | 5 103.512 | 1.00 33.23 |
| ATOM | 709 | 0 | ASN | | | 38.687 | _5 22 | 7 103.523 | 1.00 32.48 |
| MOTA | 710 | N | ILE | | 8 | _ | | , 103.3 23 | |
| | 711 | CA | | | 8 | 39.676 | | 8 104.248 | |
| ATOM | | | | | 8 | 39.030 | -6.73 | 2 105.445 | |
| MOTA √ | 712 | СВ | | | | 40.021 | | 0 106.081 | |
| ATOM | 713 | CG | | | 8 | | | 7 106.461 | |
| ATOM | 714 | CG | 1 ILE | A 8 | 8 | 38.536 | | | |
| | 715 | | | | 8 | 39.641 | -4.95 | | |
| ATOM | | | | | | 40.251 | | | 1.00 37.36 |
| ATOM | 716 | | ILE | | 8 | | | | |
| MOTA | 717 | 0 | ILE | | 8 | 39.555 | | | |
| | 718 | | GLY | | 9 | 41.517 | | | |
| MOTA | | | | | 9 | 42.124 | -8.47 | 7 102.698 | |
| MOTA | 719 | | | | | 43.134 | | | 1.00 34.50 |
| MOTA | 720 | C | GLY | | 39 | | | | |
| MOTA | 721 | . 0 | GLY | A 8 | 39 | 43.951 | | | |
| | 722 | | GLY | | 90 | 43.071 | 6.71 | | 1.00 31.33 |
| ATOM | | | | | 90 | 44.005 | | 8 100.371 | 1.00 23.90 |
| MOTA | 723 | | | | | 45.340 | | | 1.00 28.78 |
| ATOM | 724 | l C | GLY | | 90 | | | | |
| ATOM | 725 | | GLY | A ! | 90 | 45.563 | -6.33 | . 100.103 | |
| | 726 | | TYR | | 91 | 46.221 | -5.15 | 55 100.367 | 1.00 20.20 |
| MOTA | 120 | . 14 | 7 + 1 | | _ | | | | |
| | | | | | | | | | |

| | | | | | | | | 010 | 1.00 27.34 |
|------|------|------|---------|------|---|--------|----------|---------------------------------------|------------|
| ATOM | 727 | CA | TYR A | 91 | | 47.539 | | 100.918 | |
| | | | TYR A | 91 | | 48.477 | -4.365 | 99.805 | 1.00 22.62 |
| MOTA | 728 | CB | - | | | 48.066 | -3.039 | 99.194 | 1.00 24.28 |
| ATOM | 729 | CG | TYR A | 91 | | | | 99.822 | 1.00 21.55 |
| ATOM | 730 | CD1 | TYR A | 91 | | 48.374 | -1.829 | | |
| | | CEl | TYR A | 91 | | 47.970 | -0.609 | 99.275 | 1.00 24.69 |
| MOTA | 731 | | | | | 47.341 | -2.997 | 98.002 | 1.00 24.86 |
| ATOM | 732 | CD2 | TYR A | 91 | | | -1.786 | 97.447 | 1.00 29.92 |
| MOTA | 73,3 | CE2 | TYR A | 91 | | 46.931 | | | 1.00 29.04 |
| MOTA | 734 | cz | TYR A | 91 | | 47.250 | -0.597 | 98.086 | |
| | | | TYR A | 91 | | 46.861 | 0.593 | 97.516 | 1.00 29.51 |
| ATOM | 735 | OH | | | | 47.452 | -3.777 | 101.998 | 1.00 27.52 |
| MOTA | 736 | С | TYR A | 91 | | | | 102.869 | 1.00 27.20 |
| MOTA | 737 | 0 | TYR A | 91 | - | 48.314 | -3.689 | | 1.00 26.75 |
| | 738 | Ŋ | GLU A | 92 | | 46.402 | -2.971 | 101.938 | |
| ATOM | | | GLU A | 92 | | 46.232 | -1.879 | 102.882 | 1.00 28.38 |
| MOTA | 739 | CA | | | | 45.234 | -0.881 | 102.310 | 1.00 28.57 |
| MOTA | 740 | CB | GLU A | 92 | | 45.233 | 0.471 | 102.982 | 1.00 36.94 |
| ATOM | 741 | CG | GLU A | 92 | | 45.232 | | | 1.00 37.40 |
| ATOM | 742 | CD | GLU A | 92 | | 44.178 | 1.395 | 102.396 | |
| | | OE1 | | 92 | | 42.999 | 1.293 | 102.794 | 1.00 31.22 |
| MOTA | 743 | | | 92 | | 44.527 | 2.209 | 101.516 | 1.00 40.54 |
| ATOM | 744 | | GLU A | | | 45.770 | -2.343 | 104.259 | 1.00 29.20 |
| ATOM | 745 | С | GLU A | 92 | | | | 105.268 | 1.00 21.86 |
| ATOM | 746 | 0 | GLU A | 92 | | 46.389 | -2.015 | 103.200 | |
| | 747 | N | ASN A | 93 | | 44.687 | -3.117 | 104.286 | 1.00 26.51 |
| ATOM | | | | 93 | | 44.109 | -3.613 | 105.527 | 1.00 24.02 |
| MOTA | 748 | CA | ASN A | | | 42.727 | -2.988 | | 1.00 24.51 |
| ATOM | 749 | CE | ASN A | 93 | | 42.727 | -1.488 | | 1.00 28.61 |
| ATOM | 750 | CG | ASN A | 93 | | 42.738 | | | |
| | 751 | OD1 | | 93 | | 43.428 | -0.727 | 106.079 | |
| ATOM | | | | 93 | | 41.987 | -1.063 | 104.393 | 1.00 20.45 |
| MOTA | 752 | ND2 | | | | 43.999 | -5.132 | | 1.00 24.79 |
| MOTA | 753 | С | ASN A | 93 | | | -5.680 | 105.291 | 1.00 21.89 |
| ATOM | 754 | 0 | ASN A | 93 | | 42.905 | -5.000 | | |
| | 755 | N | PRO A | 94 | | 45.142 | -5.828 | 105.429 | |
| ATOM | | CD | PRO A | 94 | | 46.493 | -5.246 | | 1.00 22.93 |
| MOTA | 756 | | | | | 45.241 | -7.285 | 105.312 | 1.00 27.23 |
| MOTA | 757 | CA | PRO A | 94 | | | _7 / 200 | 105.093 | 1.00 25.46 |
| ATOM | 758 | CB | PRO A | 94 | | 46.730 | -7.400 | 105.055 | 1.00 26.20 |
| ATOM | 759 | CG | PRO A | 94 | | 47.299 | | 106.046 | 1.00 20.20 |
| | | c | PRO A | 94 | | 44.743 | -8.112 | 106.489 | 1.00 31.04 |
| ATOM | 760 | | | 94 | | 44.411 | -7.589 | 107.558 | 1.00 29.10 |
| MOTA | 761 | С | PRO A | | | 44.696 | -9.422 | | 1.00 28.27 |
| ATOM | 762 | N | VAL A | 95 | | | | | 1.00 28.82 |
| MOTA | 763 | CA | VAL A | 95 | | 44.299 | -10.367 | | 1.00 30.75 |
| | 764 | СЗ | VAL A | 95 | | 43.938 | -11.737 | 106.677 | |
| MOTA | | | | 95 | | 43.745 | -12.766 | 107.776 | 1.00 33.60 |
| MOTA | 765 | CG: | _ | | | 42.679 | -11.611 | 105.849 | 1.00 24.87 |
| MOTA | 766 | CG: | | 95 | | _ | -10.549 | 108.204 | 1.00 29.98 |
| ATOM | 767 | С | VAL A | 95 | | 45.503 | | | 1.00 31.36 |
| ATOM | 768 | 0 | VAL A | 95 | | 46.637 | -10.649 | | |
| | 769 | N | SER A | 96 | | 45.254 | -10.572 | 2 109.510 | 1.00 29.38 |
| MOTA | | | | 96 | | 46.335 | -10.766 | 110.485 | 1.00 32.56 |
| MOTA | 770 | CA | SER A | | | 47.325 | -9.600 | 110.454 | 1.00 34.15 |
| ATOM | 771 | CB | SER A | 96 | | | | | 1.00 28.33 |
| MOTA | 772 | CG | SER A | 96 | | 46 758 | -8.448 | | 1.00 32.10 |
| | 773 | С | SER A | 96 | | 45.681 | ~10.804 | 4 111.854 | 1.00 32.10 |
| ATOM | 774 | | SER A | | | 44 458 | -10.83 | 9 111.950 | 1.00 37.9 |
| ATOM | | 0 | | | | 46 484 | -10.79 | 5 112.913 | 1.00 32.5 |
| ATOM | 775 | 11 | TYR A | | | 45.014 | 10 80 | | 1.00 34.9 |
| ATOM | 776 | CA | TYR A | | • | 45.914 | -10.80 | | |
| ATOM | 777 | CЭ | TYR A | 97 | | 46.685 | -11.73 | | |
| | | | | | | 46.492 | -13.18 | 7 114.817 | |
| MOTA | 778 | | | | | 47 319 | -13.81 | 2 113.882 | 1.00 40.6 |
| ATOM | 779 | | | | | 47 003 | -15 12 | 1 113 475 | |
| ATOM | 780 | CE | 1 TYR A | | | 47.083 | -13.12 | 0 115 330 | |
| | 781 | | | 97 | | 45.421 | -13.91 | 0 115.338 | |
| MOTA | | | | | | 45.175 | -15.21 | 9 114.936 | 1.00 42.8 |
| atom | 78,2 | | | | | 46 010 | -15.81 | 6 114.005 | 1.00 42.5 |
| MOTA | 783 | | | | | 45 777 | -17.10 | | |
| ATOM | 784 | CH | TYR A | | | 40.112 | -11.10 | | |
| | 785 | | TYR A | 97 | | 45.862 | -9.39 | | |
| ATOM | | | TYR A | | | 45.501 | | 5 115.998 | 1.00 39.0 |
| ATCM | 786 | | | | | 46.115 | -841 | 8 113.948 | 1.00 31.9 |
| ATCM | 787 | | ALA A | | | | -7 02 | 4 114.341 | 1.00 30.4 |
| ATOM | 788 | 3 CA | , ALA A | | | 46.048 | | 1 113.600 | |
| | 789 | | | 98 | | 47.105 | | 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 | |
| ATOM | 790 | | ALA A | | | 44.658 | -6.53 | 3 113.962 | |
| ATOM | | | | | | 44.099 | -5.65 | 5 114.612 | 1.00 31.8 |
| ATCM | 791 | | ALA A | | | 44.094 | | 0 112.915 | 1.00 30.4 |
| ATOM | 792 | 2 N | MET A | 4 99 | | 44.034 | | | |
| | | | | | | | | | |

| | | | 42.788 | -6.730 112.420 | 1.00 27.54 |
|--------|-----|---------------|----------|-----------------|-------------|
| ATOM | 793 | CA MET A 99 | 42.700 | -7.620 111.238 | 1.00 30.55 |
| ATOM | 794 | CB MET A 99 | | -7.020 111.250 | 1.00 31.59 |
| ATOM | 795 | CG MET A 99 | 42.052 | -9.071 111.565 | |
| ATOM | 796 | SD MET A 99 | 41.902 - | 10.077 110.053 | 1.00 30.13 |
| | 797 | CE MET A 99 | 40.770 | -9.086 109.085 | 1.00 28.02 |
| MOTA | | | 41.703 | -6.696 113.490 | 1.00 28.02 |
| ATOM - | 798 | • | 40.818 | -5.842 113.446 | 1.00 24.53 |
| ATOM | 799 | O MET A 99 | | -7.614 114.449 | 1.00 26.07 |
| ATOM | 800 | N PHE A 100 | 41.752 | -7.014 114.445 | 1.00 30.47 |
| ATOM | 801 | CA PHE A 100 | 40.759 | -7.583 115.516 | 1.00 30.29 |
| | 802 | CB PHE A 100 | 39.738 | -8.718 115.404 | |
| MOTA | 803 | CG PHE A 100 | 38.693 | -8.657 116.475 | 1.00 29.35 |
| ATOM | | | 37.722 | -7.662 116.455 | 1.00 27.01 |
| MOTA | 804 | | 38.756 | -9.506 117.575 | 1.00 30.68 |
| ATOM | 805 | CD2 PHE A 100 | 36.834 | -7.507 117.519 | 1.00 31.41 |
| ATOM | 806 | CE1 PHE A 100 | | -9.356 118.644 | 1.00 28.39 |
| MOTA | 807 | CE2 PHE A 100 | | -8.355 118.618 | 1.00 24.06 |
| ATOM | 808 | CZ PHE A 100 | | -8.355 116.010 | 1.00 29.67 |
| ATOM | 809 | C PHE A 100 | 41.345 | -7.616 116.922 | 1.00 29.07 |
| MOTA | 810 | O PHE A 100 | 41.028 | -6.751 117.740 | 1.00 29.67 |
| | 811 | N THR A 101 | 42.181 | -8.610 117.222 | 1.00 31.30 |
| ATOM | | CA THR A 101 | 42.770 | -8.701 118.562 | 1.00 31.37 |
| ATOM | 812 | | 43.610 | -9.977 118.732 | 1.00 31.63 |
| MOTA | 813 | | 42.777 - | -11.119 118.532 | 1.00 31.64 |
| ATOM | 814 | OG1 THR A 101 | 44.107 | 10.045 120.137 | 1.00 27.38 |
| ATOM | 815 | CG2 THR A 101 | 44.197 | -7.493 118.884 | 1.00 31.66 |
| MOTA | 816 | C THR A 101 | 43.647 | | 1.00 30.71 |
| ATOM | 817 | O THR A 101 | 43.502 | -6.875 119.942 | 1.00 30.71 |
| MOTA | 818 | N GLY A 102 | 44.562 | -7.166 117.976 | |
| | 819 | CA GLY A 102 | 45.430 | -6.018 118.193 | 1.00 27, 19 |
| MOTA | | | 44.631 | -4.728 118.266 | 1.00 27.26 |
| MOTA | 820 | | 44.785 | -3.940 119.201 | 1.00 27.68 |
| MOTA | 821 | | 43.767 | -4.515 117.279 | 1.00 30.52 |
| ATOM | 822 | N SER A 103 | | -3.314 117.216 | 1.00 31.91 |
| ATOM | 823 | CA SER A 103 | 42.941 | -3.334 115.949 | 1.00 34.63 |
| ATOM | 824 | CB SER A 103 | 42.085 | -3.334 113.343 | 1.00 35.94 |
| ATOM | 825 | OG SER A 103 | 42.896 | -3.265 114.791 | 1.00 32.44 |
| ATOM | 826 | C SER A 103 | 42.046 | -3.163 118.441 | 1.00 32.44 |
| | 827 | O SER A 103 | 41.891 | -2.065 118.984 | 1.00 25.78 |
| ATOM | 828 | N SER A 104 | 41.455 | -4.270 118.871 | 1.00 30.47 |
| ATOM | | CA SER A 104 | 40.584 | -4.251 120.038 | 1.00 30.22 |
| ATOM | 829 | | 39.978 | -5.633 120.265 | 1.00 23.88 |
| MOTA | 830 | CB SER A 104 | 39.078 | -5.595 121.358 | 1.00 36.91 |
| ATOM | 831 | OG SER A 104 | 41.367 | -3.841 121.282 | 1.00 28.13 |
| ATOM | 832 | C SER A 104 | | -3.098 122.130 | 1.00 25.16 |
| ATOM | 833 | O SER À 104 | 40.872 | -4.336 121.386 | 1.00 29.39 |
| ATOM | 834 | N LEU A 105 | 42.594 | -4.336 121.380 | 1.00 29.52 |
| ATOM | 835 | CA LEU A 105 | 43.445 | -4.034 122.530 | 1.00 32.90 |
| ATOM | 836 | CB LEU A 105 | 44.684 | -4.922 122.471 | 1.00 32.30 |
| | 837 | CG LEU A 105 | 45.461 | -5.176 123.754 | 1.00 40.34 |
| ATOM | | CD1 LEU A 105 | 44.520 | -5.723 124.828 | 1.00 35.95 |
| MOTA | 838 | CD2 LEU A 105 | 46.582 | -6.178 123.462 | 1.00 40.23 |
| MOTA | 839 | CD2 LEU A 103 | 43.834 | -2.552 122.511 | 1.00 32.09 |
| MOTA | 840 | C LEU A 105 | 43.896 | -1.894 123.554 | 1.00 30.38 |
| ATOM | 841 | O LEU A 105 | | | 1.00 30.26 |
| ATOM | 842 | N ALA A 106 | 44.081 | | 1.00 28.31 |
| ATOM | 843 | CA ALA A 106 | 44.448 | -0.626 121.151 | 1.00 23.88 |
| | 844 | CB ALA A 106 | 44.958 | -0.386 119.738 | |
| MOTA | 845 | C ALA A 106 | 43.243 | 0.268 121.434 | 1.00 26.04 |
| MOTA | | | 43.380 | 1.376 121.952 | 1.00 20.63 |
| MOTA | 846 | | 42.058 | -0.224 121.099 | 1.00 26.86 |
| ATOM | 847 | N THR A 107 | 40.841 | 0.542 121.322 | 1.00 25.04 |
| MOTA | S48 | CA THR A 107 | | 0.007 120.443 | |
| ATOM | 349 | CB THR A 107 | 39.706 | | |
| ATOM | 850 | OG1 THR A 107 | 40.111 | | |
| ATOM | 851 | CG2 THR A 107 | 38.439 | 0.824 120.629 | |
| | 352 | C THR A 107 | 40.450 | 0.503 122.798 | |
| ATOM | 352 | O THR A 107 | 40.039 | 1.515 123.361 | |
| ATOM | | | 40.585 | -0.662 123.422 | |
| MOTA | 854 | | 40.256 | -0.767 124.832 | 1.00 24.86 |
| ATOM | 855 | | 41.181 | 0.155 125.603 | 1.00 23.86 |
| ATOM | 856 | | 40.771 | 0.790 126.572 | 1.00 26.97 |
| ATCM | 857 | O GLY A 108 | | 0.790 125.372 | 1.00 23.07 |
| ATCM | 358 | N SER A 109 | 42.434 | 0.236 123.130 | |
| | | | | | |

| | | | | | | | 1 00 00 00 |
|-------|------|------|--------------|--------|--------|-----------|------------|
| 5 mow | 859 | CA | SER A 109 | 43.421 | 1.090 | 125.807 | 1.00 20.96 |
| ATOM | | | | 44.795 | 0.910 | 125.160 | 1.00 24.84 |
| ATOM | 860 | CB | SER A 109 | | -0.393 | 125.402 | 1.00 25.84 |
| ATOM | 861 | OG | SER A 109 | 45.294 | | | |
| | 862 | С | SER A 109 | 43.008 | | 125.759 | 1.00 21.13 |
| MOTA | | | | 43.323 | 3.312 | 126.672 | 1.00 23.17 |
| ATOM | 863 | 0 | SER A 109 | 40.000 | 2 949 | 124.698 | 1.00 20.83 |
| ATOM | 864 | N | THR A 110 | 42.311 | | 124.000 | |
| | 865 | CA | THR A 110 | 41.841 | 4.327 | 124.583 | 1.00 21.84 |
| MOTA | | | | 41.332 | 4.648 | 123.161 | 1.00 24.33 |
| ATOM | 866 | CB | THR A 110 | 41.352 | | 122.276 | 1.00 25.38 |
| MOTA | 867 | OG1 | THR A 110 | 42.452 | | | |
| | 868 | CG2 | THR A 110 | 40.543 | 5.954 | 123.144 | 1.00 21.18 |
| ATOM | | | | 40.725 | 4.561 | 125.600 | 1.00 28.52 |
| ATOM | 869 | С | THR A 110 | | | 126.197 | 1.00 28.27 |
| ATOM | 870 | 0 | THR A 110 | 40.632 | 5.637 | | 1.00 26.88 |
| ATOM | 871 | N | VAL A 111 | 39.882 | 3.558 | 125.809 | 1.00 26.88 |
| | | | VAL A 111 | 38.811 | 3.706 | 126.793 | 1.00 30.04 |
| MOTA | 872 | CA | VAL A III | 37.820 | 2.519 | 126.742 | 1.00 29.94 |
| ATOM | 873 | CB | VAL A 111 | | | 127.802 | 1.00 27.07 |
| ATOM | 874 | CG1 | VAL A 111 | 36.737 | 2.693 | | 1.00 27.07 |
| | 875 | CC2 | VAL A 111 | 37.193 | 2.431 | 125.355 | 1.00 25.26 |
| ATOM | | | VAD 7. 111 | 39.440 | 3.797 | 128.187 | 1.00 28.10 |
| ATOM | 876 | С | VAL A 111 | | 4.539 | 129.039 | 1.00 26.06 |
| MOTA | 877 | 0 | VAL A 111 | 38.968 | | _ | 1.00 23.92 |
| ATOM | 878 | N | GLN A 112 | 40.521 | 3.056 | | |
| | | | GLN A 112 | 41.188 | 3.097 | 129.711 | 1.00 30.27 |
| MOTA | 879 | CA | | | | 129.804 | 1.00 28.61 |
| MOTA | 880 | CB | GLN A 112 | 42.268 | 2.020 | 120.004 | 1.00 28.90 |
| ATOM | 881 | CG | GLN A 112 | 41.777 | 0.629 | 129.481 | |
| | | CD | GLN A 112 | 42.883 | -0.397 | 129.564 | 1.00 28.60 |
| ATOM | 882 | | | 43.344 | -0 740 | 130.653 | 1.00 29.68 |
| ATOM | 883 | OE1 | | | 0.720 | 128.409 | 1.00 22.13 |
| ATOM | 884 | NE2 | GLN A 112 | 43.333 | | | |
| | 885 | C | GLN A 112 | 41.834 | 4.461 | 129.931 | 1.00 29.99 |
| MOTA | | | | 41.791 | 5.006 | 131.035 | 1.00 28.43 |
| MOTA | 886 | 0 | GLN A 112 | | 5.000 | 128.885 | 1.00 28.64 |
| MOTA | 887 | N | ALA A 113 | 42.453 | 5.004 | 120.005 | 1.00 26.62 |
| ATOM | 888 | CA | ALA A 113 | 43.083 | 6.315 | 129.001 | |
| | | | ALA A 113 | 43.693 | 6.732 | 127.684 | 1.00 23.49 |
| MOTA | 889 | CB | ALA A 113 | 42.005 | 7.307 | | 1.00 24.63 |
| MOTA | 890 | С | ALA A 113 | | | | 1.00 26.38 |
| ATOM | 891 | 0 | ALA A 113 | 42.232 | 8.183 | | |
| | 892 | N | ILE A 114 | 40.824 | 7.163 | 128.822 | 1.00 25.26 |
| ATOM | | | ILE A 114 | 39.728 | 8.063 | 129.145 | 1.00 27.05 |
| MOTA | 893 | CA | | | 7.887 | | 1.00 26.93 |
| ATOM | 894 | CB | ILE A 114 | 38.554 | | | 1.00 25.86 |
| ATOM | 895 | CG2 | ILE A 114 | 37.387 | 8.770 | 128.576 | |
| | | CG1 | | 39.008 | 8.259 | 126.739 | 1.00 28.38 |
| MOTA | 896 | | | 37.938 | ន 105 | 125.669 | 1.00 28.64 |
| ATOM | 897 | CD1 | | | 7 000 | 130.578 | 1.00 31.36 |
| ATOM | 898 | С | ILE A 114 | 39.239 | | | 1.00 24.56 |
| MOTA | 899 | 0 | ILE A 114 | 38.898 | | 131.291 | |
| | | | GLU A 115 | 39.210 | 6.563 | 3 131.005 | 1.00 31.17 |
| ATOM | 900 | 1.1 | | 38.750 | 6 25" | 7 132.358 | 1.00 32.12 |
| ATOM | 901 | CA | GLU A 115 | | 4.74 | 1 132.607 | 1.00 32.15 |
| ATOM | 902 | CB | GLU A 115 | 38.729 | | | |
| | 903 | CG | GLU A 115 | 37.904 | 3.94 | | 1.00 32.84 |
| ATOM | | | GLU A 115 | 37.875 | 2.459 | 9 131.912 | 1.00 34.12 |
| ATOM | 904 | CD | | | 1 01 | 132.345 | 1.00 30.36 |
| ATOM | 905 | OE: | 1 GLU A 115 | 38.910 | | 132.010 | 1.00 31.38 |
| ATOM | 906 | OE. | 2 GLU A 115. | 36.826 | 1.82 | | 1.00 31.50 |
| | | | GLU A 115 | 39.675 | 6.93 | 2 133.357 | 1.00 31.65 |
| ATOM | 907 | С | GHU H 117 | 39.224 | 7.44 | 6 134.383 | 1.00 29.25 |
| ATOM | 908 | 0 | GLU A 115 | | 6 03 | 3 133.053 | |
| ATOM | 909 | N | GLU A 116 | 40.970 | | | 1.00 32.34 |
| | 910 | CA | | 41.942 | 7.56 | 4 133.934 | 1.00 32.34 |
| ATOM | | | GLU A 116 | 43.367 | 7.28 | 5 133.457 | 1.00 33.29 |
| ATOM | 911 | СВ | | | 5 9/ | 2 133.633 | 1.00 32.29 |
| ATOM | -912 | CG | GLU A 116 | 43.805 | | | 1.00 36.87 |
| | 913 | CD | | 43.701 | 5.37 | 8 135.079 | |
| ATOM | | | 1 GLU A 116 | 44.329 | 6.00 | 3 135.961 | |
| ATOM | 914 | | T GDO W 110 | 42.993 | 4.38 | 5 135.335 | 1.00 35.00 |
| ATOM | 915 | OE | | | | | |
| ATOM | 916 | С | GLU A 116 | 41.702 | 9.06 | | 1 00 34 30 |
| | 917 | | GLU A 116 | 41.863 | 9.67 | | |
| ATOM | | | | 41.317 | 9.66 | 1 132.881 | 1.00 31.19 |
| ATOM | 918 | N | PHE A 117 | | | | 1.00 28.43 |
| ATOM | 919 | CA | PHE A 117 | 41.038 | | | |
| | 920 | | | 40.593 | 11.50 | | |
| ATOM | | | | 40.044 | | 8 131.381 | 1.00 35.78 |
| ATOM | 921 | . CG | FRE A 11/ | 40.882 | | 6 131.501 | 1.00 33.39 |
| ATOM | 922 | CD | 1 PHE A 117 | | | | |
| ATOM | 923 | CD | 2 PHE A 117 | 38.675 | | | |
| | 924 | | 1 PHE A 117 | 40.372 | 15.29 | 9 131.466 | 1.00 20.02 |
| ATOM | 744 | . CE | | | | | |
| | | | | | | | |

| MOTA | 925 | CE2 F | HE A 117 | | 38.153 | 14.412 | 131.190 | 1.00 36.50 |
|--------------|------------|----------|------------------------|---|------------------|----------------|------------------------|--------------------------|
| | 926 | CZ F | HE A 117 | | 39.003 | | 131.310 | 1.00 35.41 1.00 32.78 |
| ATOM | 927 | | PHE A 117 | | 39.908 | | 133.811 134.566 | 1.00 32.78 |
| ATOM | 928 | | PHE A 117 | | 39.966 | 12.3// | 134.500 | 1.00 28.61 |
| ATOM | 929 | | EU A 118 | | 38.874 | 10.751 | 134.632 | 1.00 32.00 |
| ATOM | 930 | | EU A 118 | | 37.720 | | 134.263 | 1.00 29.19 |
| MOTA | 931 | | LEU A 118 | | 36.621 36.098 | | 132.820 | 1.00 34.47 |
| ATOM | 932 | | LEU A 118 | | 34.962 | | 132.622 | 1.00 32.69 |
| MOTA | 933 | CD1 L | LEU A 118 | | 35.612 | 11.240 | 132.522 | 1.00 32.24 |
| ATOM | 934 | CD2 I | LEU A 118 LEU A 118 | | 38.123 | 10.590 | 136.094 | 1.00 31.17 |
| MOTA | 935 | C I | LEU A 118 | | 37.576 | 11.260 | 136.964 | 1.00 28.32 |
| MOTA | 936 937 | N I | LYS A 119 | | 39.083 | 9.707 | 136.363 | 1.00 27.23 |
| MOTA MOTA | 938 | CA I | LYS A 119 | | 39.531 | 9.497 | 137.733 | 1.00 30.95 |
| ATOM | 939 | CB I | LYS A 119 | | 40.203 | 8.130 | 137.884 | 1.00 26.35 |
| ATOM | 940 | CG I | LYS A 119 | | 39.293 | 6.954 | 137.540 | 1.00 32.44 1.00 33.31 |
| MOTA | 941 | | LYS A 119 | | 39.895 | 5.624 | 137.986 137.411 | 1.00 33.31 |
| ATOM | 942 | CE I | LYS A 119 | | 41.280 | 5.383 4 103 | 137.904 | 1.00 33.40 |
| ATOM | 943 | | LYS A 119 | | 41.874 40.493 | 10 594 | 138.173 | 1.00 32.65 |
| ATOM | 944 | C I | LYS A 119 | • | 40.453 | 10.534 | 139.270 | 1.00 28.83 |
| MOTA | 945 | 0 | LYS A 119 | | 40.689 | 11.583 | 137.308 | 1.00 33.77 |
| MOTA | 946 | N (| GLY A 120 GLY A 120 | | 41.571 | 12.677 | 137.652 | 1.00 33.84 |
| MOTA | 947 | CA (| GLY A 120 | | 43.035 | 12.448 | 137.340 | 1.00 34.27 |
| ATOM | 948 949 | 0 | GLY A 120 | | 43.880 | 13.227 | 137.776 | 1.00 36.80 |
| ATOM | 950 | N . | ASN A 121 | | 43.347 | 11.384 | 136.606 | 1.00 30.77 |
| MOTA MOTA | 951 | CA | ASN A 121 | | 44.731 | 11.122 | 136.244 | 1.00 31.73 |
| MOTA | 952 | CB . | ASN A 121 | | 45.089 | 9.646 | 136.437 | 1.00 29.34 1.00 35.83 |
| ATOM | 953 | CG | ASN A 121 | | 44.856 | 9.170 | 137.851 | 1.00 33.83 |
| ATOM | 954 | OD1 | ASN A 121 | | 45.190 | 9.861 | 138.816 137.986 | 1.00 33.20 |
| MOTA | 955 | | ASN A 121 | | 44.304 | 11 506 | 134.790 | 1.00 32.59 |
| MOTA | 956 | | ASN A 121 | | 44.954 44.031 | 11 952 | 134.110 | 1.00 34.69 |
| MOTA | 957 | 0 | ASN A 121 | | 46.186 | 11:334 | 134.322 | 1.00 32.74 |
| MOTA | 958 | N | VAL A 122 VAL A 122 | | 46.540 | 11.653 | 132.946 | 1.00 33.59 |
| ATOM | 959 960 | CA CB | VAL A 122 | | 47.571 | 12.790 | 132.882 | 1.00 36.05 |
| MOTA | 961 | CG1 | VAL A 122 | | 47.884 | 13.121 | 131.438 | 1.00 37.58 |
| MOTA MOTA | 962 | CG2 | VAL A 122 | | 47.029 | 14.021 | 133.602 | 1.00 37.19 1.00 34.47 |
| ATOM | 963 | С | VAL A 122 | | 47.147 | 10.397 | 132.352 | 1.00 34.47 |
| ATOM | 964 | 0 | VAL A 122 | | 48.053 | 9.801 | 132.939 | 1.00 28.06 |
| ATOM | 965 | N | ALA A 123 | | 46.646 | 9.303 | 130.563 | 1.00 30.73 |
| ATOM | 966 | CA | ALA A 123 | | 47.142 46.133 | 7 666 | 130.727 | 1.00 32.69 |
| ATOM | 967 | CB | ALA A 123 ALA A 123 | | 47.466 | 8.969 | 129.088 | 1.00 30.55 |
| MOTA | 968 | C | ALA A 123 | | 46.909 | 9.830 | 128.406 | 1.00 32.89 |
| MOTA | 969 970 | N 0 | PHE A 124 | | 48.380 | 8.130 | 5 128.613 | 1.00 27.53 |
| ATOM | 971 | CA | PHE A 124 | | 48.807 | 8.15 | 7 127.229 | 1.00 26.56 |
| MOTA MOTA | 972 | CB | PHE A 124 | | 50.261 | | 127.157 | 1.00 25.32 1.00 27.84 |
| ATOM | 973 | CG | PHE A 124 | | 50.903 | 8.54 | 4 125.793 | 1.00 24.77 |
| ATOM | 974 | CD1 | PHE A 124 | | 50.179 | 8.78 | 5 124.629 | |
| ATOM | 975 | CD2 | PHE A 124 | | 52.266 | 8.25 | 6 125.686 3 123.385 | |
| ATOM | 976 | CE1 | PHE A 124 | | 50.802 | 8.73 | | |
| ATOM | 977 | | PHE A 124 | | 52.894 52.164 | 8.47 | | |
| ATOM | 978 | | PHE A 124 | | 48.671 | 6.74 | 9 126.675 | 1.00 21.13 |
| MOTA | 979 | | PHE A 124 | | 49.181 | 5.79 | | 1.00 25.38 |
| ATOM | 980 | | PHE A 124 ASN A 125 | | 47.933 | 6.62 | 4 125.580 | 1.00 18.87 |
| ATOM | 981 | | ASN A 125 | | 47.750 | 5.34 | | 1.00 25.05 |
| ATOM | 982 983 | | ASN A 125 | | 46.271 | 4.98 | 2 124.756 | |
| ATOM | 984 | | ASN A 125 | | 46.073 | 3.78 | 4 123.856 | 1.00 24.08 |
| ATOM TOM | 985 | | ASN A 125 | | 46.916 | | | |
| atom atom | 986 | | ASN A 125 | | 44.960 | | | |
| ATOM | 987 | | ASN A 125 | | 48.380 | | | |
| ATOM | 988 | | ASN A 125 | | 47.718 | | | |
| ATOM | 989 | | PRO A 126 | | 49.680 | | 0 124.519 | |
| ATOM | 990 | CD (C | PRO A 126 | | 50.589 | 4.73 | | |
| | | | | | | | | |

| | | | | 100 160 | 1.00 22.39 |
|------|-------|-----------------|----------|----------------|------------|
| ATOM | 991 | CA PRO A 126 | 50.413 | 5.130 122.160 | |
| | | CB PEO A 126 | 51.829 | 4.751 122.594 | 1.00 18.20 |
| ATOM | | | 51.564 | 3.849 123.798 | 1.00 25.43 |
| ATOM | | CG PRO A 126 | | 4.224 121.058 | 1.00 23.18 |
| ATOM | 994 | C PRO A 126 | 49.867 | 4.224 121.000 | 1.00 20.12 |
| ATOM | 995 | O PRO A 126 | 50.173 | 4.436 119.893 | |
| | | N ALA A 127 | 49.058 | 3.232 121.423 | 1.00 23.27 |
| ATOM | | N ALA A 12. | 48.493 | 2.306 120.444 | 1.00 23.89 |
| ATOM | 997 | CA ALA A 127 | | 0.967 121.118 | 1.00 24.82 |
| MOTA | 998 | CB ALA A 127 | 48.176 | | 1.00 24.76 |
| ATOM | | C ALA A 127 | 47.241 | 2.864 119.778 | |
| | | 107 | 46.806 | 2.360 118.745 | 1.00 28.99 |
| MOTA | | O ALA A 12/ | . 46.666 | 3.906 120.367 | 1.00 22.12 |
| MOTA | 1001 | N GLY A 128 | | 4.494 119.809 | 1.00 21.43 |
| ATOM | 1002 | CA GLY A 128 | 45.461 | 4.494 119.005 | 1.00 23.55 |
| ATOM | 1003 | C GLY A 128 | 45.732 | 5.521 118.725 | 1.00 23.35 |
| | 1004 | O GLY A 128 | 46.875 | 5.695 118.291 | 1.00 23.25 |
| ATOM | | | 44.680 | 6.199 118.283 | 1.00 18.03 |
| ATOM | 1005 | N GLY A 129 | 44.822 | 7.205 117.243 | 1.00 24.99 |
| MOTA | 1006 | CA GLY A 129 | | | 1.00 25.11 |
| MOTA | 1007 | C GLY A 129 | 44.600 | | 1.00 24.99 |
| ATOM | 1008 | O GLY A 129 | 44.963 | 7.293 114.857 | 1.00 24.33 |
| | | | 44.002 | 5.470 115.765 | 1.00 20.01 |
| MOTA | 1009 | N MET A 130 | 43.729 | 4.825 114.481 | 1.00 23.63 |
| MOTA | 1010 | CA MET A 130 | | 3.361 114.744 | 1.00 22.77 |
| ATOM | 1011 | CB MET A 130 | 43.360 | 3.301 114.717 | 1.00 26.30 |
| ATOM | 1012 | CG MET A 130 | 44.455 | 2.661 115.563 | 1.00 20.50 |
| | - | SD MET A 130 | 44.198 | 0.913 115.989 | 1.00 26.57 |
| ATOM | 1013 | 5D FET A 130 | 42.665 | 1.030 116.936 | 1.00 27.59 |
| MOTA | 1014 | CE MET A 130 | 42.580 | 5.617 113.869 | 1.00 23.70 |
| ATOM | 1015 | C MET A 130 | | 5.199 113.901 | 1.00 26.28 |
| ATOM | 1016 | O MET A 130 | 41.421 | 5.199 113.901 | 1.00 20.66 |
| | 1017 | N HIS A 131 | 42.926 | 6.766 113.294 | 1.00 20.00 |
| MOTA | | | 41.933 | 7.687 112.775 | 1.00 20.99 |
| MOTA | 1018 | CA HIS A 131 | 42.474 | 9.125 112.891 | 1.00 21.01 |
| MOTA | 1019 | CB HIS A 131 | | 9.391 112.069 | 1.00 28.30 |
| MOTA | 1020 | CG HIS A 131 | 43.699 | 9.391 112.003 | 1.00 19.65 |
| | 1021 | CD2 HIS A 131 | 44.498 | 8.549 111.373 | 1.00 19.05 |
| ATOM | | ND1 HIS A 131 | 44.246 | 10.649 111.917 | 1.00 27.76 |
| MOTA | 1022 | NDI NIS A ISI | 45.328 | 10.567 111.163 | 1.00 20.48 |
| ATOM | 1023 | CE1 HIS A 131 | | 9.302 110.820 | 1.00 24.18 |
| ATOM | 1024 | NE2 HIS A 131 . | 45.503 | 7.513 111.416 | 1.00 23.76 |
| MOTA | 1025 | C HIS A 131 | 41.280 | /.513 111.410 | |
| | 1026 | O HIS A 131 | 40.453 | 8.341 111.051 | 1.00 21.93 |
| MOTA | | | 41.600 | 6.449 110.682 | 1.00 25.12 |
| MOTA | 1027 | N HIS A 132 | 41.006 | 6.257 109.354 | 1.00 23.32 |
| MOTA | 1028 | CA HIS A 132 | | 5.715 108.388 | 1.00 17.87 |
| MOTA | 1029 | CB HIS A 132 | 42.060 | 5.715 108.500 | 1.00 24.79 |
| ATOM | 1030 | CG HIS A 132 | 43.148 | 6.689 108.072 | 1.00 24.72 |
| | 1031 | CD2 HIS A 132 | 44.496 | 6.574 108.144 | 1.00 21.72 |
| ATOM | | ND1 HIS A 132 | 42.896 | 7.944 107.556 | 1.00 13.58 |
| MOTA | 1032 | NDI HIS A 132 | 44.044 | 8.558 107.323 | 1.00 15.41 |
| ATOM | 1033 | CE1 HIS A 132 | | 7.748 107.668 | 1.00 15.27 |
| MOTA | 1034 | NE2 HIS A 132 | 45.028 | 7.748 107.000 | 1.00 23.38 |
| MOTA | 1035 | C HIS A 132 | 39.752 | 5.386 109.208 | |
| | | | 38.947 | 5.615 108.304 | 2 00 24.70 |
| MOTA | 1036 | 0 HIS A 132 | 39.587 | 4.388 110.070 | 1.00 23.34 |
| MOTA | 1037 | N ALA A 133 | | 3.471 109.953 | 1 00 23.77 |
| ATOM | 1038 | CA ALA A 133 | 38.453 | 3.471 103.555 | 1.00 27.49 |
| ATOM | 1039 | CB ALA A 133 | 38.515 | 2.417 111.053 | |
| | 1040 | C ALA A 133 | 37.093 | 4.145 109.966 | 1.00 23.02 |
| ATOM | | | 36.878 | 5.117 110.691 | 1.00 25.98 |
| MOTA | 1041 | 0 ALA A 133 | 36.179 | 3.633 109.148 | 1.00 18.90 |
| ATOM | 1042 | N PHE A 134 | | 4.173 109.103 | |
| MOTA | 1043 | CA PHE A 134 | < 34.831 | 4.1/3 109.103 | |
| | 1044 | CB PHE A 134 | 34.317 | 4.296 107.663 | |
| MOTA | | | 35.119 | 5.225 106.801 | 1.00 26.67 |
| MOTA | 1045 | | 36.025 | 4.724 105.867 | 1.00 28.69 |
| MOTA | 1046 | CD1 PHE A 134 | | 6.605 106.921 | |
| ATOM | 1047 | CD2 PHE A 134 | 34.975 | 0.003 100.321 | |
| | 1048 | CE1 PHE A 134 | 36.775 | 5.582 105.063 | |
| ATOM | | | 35.724 | 7.479 106.119 | 1.00 27.86 |
| ATOM | 1049 | | 36.623 | 6.967 105.188 | 1.00 23.93 |
| ATOM | 1050 | CZ PHE A 134 | 30.023 | 3.260 109.884 | |
| ATOM | 1051 | C PHE A 134 | 33.894 | | |
| ATOM | 1052 | O PHE A 134 | 34.270 | 2.172 110.319 | |
| | | N LYS A 135 | 32.670 | 3.728 110.062 | |
| MOTA | 1053 | 135 | 31.638 | 2.984 110.765 | 1.00 35.26 |
| ATCM | 1054 | CA LYS A 135 | 30.294 | 3.628 110.429 | 1.00 35.86 |
| ATOM | 1055 | CB LYS A 135 | | 2.779 110.667 | |
| ATOM | 1056 | CG LYS A 135 | 29.072 | 2.113 110.00 | . |
| C11 | _,,,, | | | | |

| | | | | - | -6 | | | | |
|--------------|--------------|------------|------------------------|---|------------------|------------------|------------------------|------------------|----------------|
| ATOM | 1057 | CD L | YS A 135 YS A 135 | | 27.834 26.610 | 2.645 | 110.211 110.169 | 1.00 4 1.00 5 | 3.65 |
| MOTA | 1058 | | YS A 135 | | 26.788 | | 109.167 | 1.00 5 | |
| ATOM | 1059 1060 | | YS A 135 | | 31.617 | | 110.414 | 1.00 3 | |
| MOTA MOTA | 1061 | O L | YS A 135 | | 31.609 | | 111.301 | 1.00 3 1.00 3 | |
| ATOM- | 1062 | N S | ER A 136 | | 31.629 | 1.180 | 109.122 | 1.00 3 | |
| ATOM | 1063 | CA S | ER A 136 | | | -0.211 | 108.684 | 1.00 3 | |
| ATOM | 1064 | | ER A 136 | | 30.172 | -0.474 -0.072 | | 1.00 4 | |
| ATOM | 1065 | | ER A 136 | | 29.146 32.608 | -0.616 | 107.660 | 1.00 3 | 7.84 |
| ATCM | 1066 | C -S | ER A 136 ER A 136 | | 32.350 | | 106.828 | 1.00 3 | 6.33 |
| MOTA | 1067 | 0 S | RG A 137 | | 33.788 | -0.008 | 107.705 | 1.00 3 | |
| ATOM ATOM | 1068 1069 | N A | RG A 137 | • | 34.797 | -0.368 | 106.724 | 1.00 3 | |
| ATOM | 1070 | CB A | ARG A 137 | | 34.456 | 0.291 | 105.385 | 1.00 3 | |
| MOTA | 1071 | | ARG A 137 | | 35.009 | 0.261 | 104.201 102.880 | 1.00 4 | 6.27 |
| ATOM | 1072 | | ARG A 137 | | 34.809 35.091 | | 101.768 | 1.00 4 | |
| MOTA | 1073 | NE A | ARG A 137 ARG A 137 | | 35.352 | -0.261 | 100.526 | 1.00 4 | 18.64 |
| MOTA | 1074 1075 | CZ A | ARG A 137 | | 35.372 | 1.029 | 100.220 | 1.00 | |
| ATOM | 1075 | NH2 A | ARG A 137 | | 35.592 | -1.169 | 99.589 | 1.00 | 19.01 |
| MOTA MOTA | 1077 | | ARG A 137 | | 36.209 | 0.021 | 107.143 | 1.00 | 31.04 |
| ATOM | 1078 | 0 7 | ARG A 137 | | 36.428 | 1.079 | 107.742 106.828 | 1.00 | 30.30 |
| ATOM | 1079 | | ALA A 138 | | 37.166 38.560 | -0.845 | 100.020 | 1.00 | |
| MOTA | 1080 | | ALA A 138 | | 39.367 | -1.864 | 107.048 | 1.00 | 31.25 |
| MOTA | 1081 | CB 2 | ALA A 138 ALA A 138 | | 39.095 | 0.449 | 106.187 | 1.00 | 29.49 |
| ATOM | 1082 1083 | 0 1 | ALA A 138 | | 38.612 | 0.551 | 105.063 | 1.00 | 26.11 |
| ATOM ATOM | 1084 | N | ASN A 139 | | 40.099 | 1.206 | 106.615 | 1.00 | 29.54 26 99 |
| ATOM | 1085 | CA I | ASN A 139 | | 40.673 | 2.241 | 105.767 105.662 | 1.00 | 24.10 |
| MOTA | 1086 | CB . | ASN A 139 | | 39.685 | 4 556 | 104.811 | 1.00 | 28.02 |
| MOTA | 1087 | CG . | ASN A 139 | | 40.209 | 4.334 | 103.727 | 1.00 | 26.90 |
| MOTA | 1088 | ND2 | ASN A 139 ASN A 139 | | 40.050 | 5.789 | 105.293 | 1.00 | 23.55 |
| ATOM | 1089 1090 | C | ASN A 139 | | 42.027 | 2.713 | 106.285 | 1.00 | 30.17 |
| ATOM ATOM | 1091 | o l | ASN A 139 | | 42.245 | 2.827 | 107.497 | 1.00 | 27.55 31.82 |
| ATOM | 1092 | N | GLY A 140 | | 42.944 | 2.959 | 105.354 105.702 | | 24.90 |
| ATOM | 1093 | | GLY A 140 | | 44.277 45.000 | 2.696 | 106.816 | 1.00 | 27.79 |
| ATOM | 1094 | | GLY A 140 GLY A 140 | | 45.560 | 3.339 | 107.705 | 1.00 | 23.85 |
| MOTA | 1095 1096 | | PHE A 141 | | 45.006 | 1.365 | 106.768 | 1.00 | 24.35 |
| MOTA MOTA | 1097 | CA | PHE A 141 | | 45.679 | 0.538 | | 1.00 | 24.53 26.40 |
| ATOM | 1098 | CB | PHE A 141 | | 47.031 | 1.146 | | 1.00 | 30.31 |
| ATOM | 1099 | CG | PHE A 141 | | 47.997 49.145 | 1.366 | | 1.00 | 31.60 |
| MOTA | 1100 | CD1 | PHE A 141 | | 47.781 | 0.811 | 105.802 | 1.00 | 29.44 |
| MOTA | 1101 | CD2 | PHE A 141 PHE A 141 | | 50.066 | 2.331 | 106.243 | 1.00 | 30.44 |
| MOTA | 1102 1103 | CE1 CE2 | PHE A 141 | | 48.694 | 1.008 | 3 104.770 | | 27.91 |
| MOTA ATOM | 1103 | | PHE A 141 | | 49.840 | | 104.991 | | 29.38 23.53 |
| MOTA | 1105 | | PHE A 141 | | 44.846 | 0.387 | 7 109.056 9 109.941 | | 23.09 |
| MOTA | 1106 | | PHE A 141 | | 45.194 43.760 | 1.14 | | | 22.86 |
| MOTA | 1107 | | CYS A 142 | | 42.925 | 1.099 | 110.356 | 1.00 | 23.87 |
| ATOM | 1108 | | CYS A 142 CYS A 142 | | 42.472 | 2.51 | 6 110.723 | 1.00 | 22.51 |
| MOTA | 1109 1110 | | CYS A 142 | | 43.828 | 3.68 | 3 111.072 | 1.00 | 27.62 |
| MOTA MOTA | 1111 | | CYS A 142 | | 41.694 | 0.20 | 5 110.233 | | 24.20 24.12 |
| ATOM | 1112 | | CYS A 142 | | 40.932 | 0.30 | | | 23.84 |
| MOTA | 1113 | N | TYR A 143 | | 41.498 | -0.66 | 6 111.236 | | 26.07 |
| MOTA | 1114 | | TYR A 143 | | 40.335 40.728 | | | 1.00 | 27.89 |
| MOTA | 1115 | | TYR A 143 TYR A 143 | | 41.829 | -3.58 | 2 110.855 | 1.00 | 27.30 |
| ATOM | 1116 | | | | 43.169 | -3.32 | 9 111.137 | 1.00 | 25.76 |
| MOTA | 1117 | CE1 | TYR A 143 | | 44.185 | -3.87 | 5 110.346 | 1.00 | 25.77 25.87 |
| atom atom | 1119 | | TYR A 143 | | 41.526 | | 4 109.762 | | 23.10 |
| ATOM | 1120 | | TYR A 143 | 1 | 42.531 | | 1 108.967 9 109.262 | 1.00 | 22.93 |
| ATOM | 1123 | ı cz | TYR A 143 | | 43.854 44.849 | | 7 108.47 | | 20.64 |
| ATOM | 1123 | 2 OH | TYR A 143 | • | 44.043 | -3.41 | === | - | |

| | | | | - • | 9 | | | |
|--------|------|------|-------------|-----|--------|--------|-----------|------------|
| | | | | | 39.281 | _0 991 | 112.193 | 1.00 24.56 |
| ATOM | 1123 | C | TYR A 143 | | 38.085 | -1 030 | 111.905 | 1.00 24.88 |
| MCTA | 1124 | 0 | TYR A 143 | | | -1.030 | 113.331 | 1.00 23.77 |
| ATOM | 1125 | N | ILE A 144 | | 39.734 | -0.4/1 | 114 735 | 1.00 27.11 |
| ATOM | 1126 | CA | ILE A 144 | | 38.833 | 0.102 | 114.335 | 1.00 24.56 |
| ATOM | 1127 | CB | ILE A 144 | | 38.871 | -0.729 | 115.643 | 1.00 24.50 |
| | 1128 | | ILE A 144 | | 37.941 | -0.120 | 116.690 | 1.00 23.47 |
| ATOM | | | ILE A 144 | | 38.430 | -2.169 | 115.346 | 1.00 28.51 |
| ATOM | 1129 | | | | 38.535 | -3.113 | 116.539 | 1.00 28.70 |
| ATOM | 1130 | | ILE A 144 | | 39.248 | 1 550 | 114.627 | 1.00 24.15 |
| MOTA | 1131 | C | ILE A 144 | | 40.428 | 1.843 | | 1.00 24.42 |
| MOTA | 1132 | 0 | ILE A 144 | | | | 114.669 | 1.00 22.04 |
| ATOM . | 1133 | N | ASN A 145 | | 38.277 | | | 1.00 21.31 |
| ATOM | 1134 | CA | ASN A 145 | | 38.555 | 3.866 | | 1.00 18.87 |
| ATOM | 1135 | CB | ASN A 145 | | 37.559 | 4.732 | | 1.00 22.21 |
| ATOM | 1136 | CG | ASN A 145 | | 37.956 | 6.205 | | |
| | 1137 | | ASN A 145 | | 38.223 | 6.823 | 115.124 | 1.00 22.47 |
| MOTA | 1138 | NID2 | ASN A 145 | | 37.978 | 6.776 | 112.892 | 1.00 23.78 |
| ATOM | | | ASN A 145 | | 38.417 | | 116.418 | 1.00 22.63 |
| ATOM | 1139 | C | ASN A 145 | | 37.338 | 4.535 | 116.880 | 1.00 22.45 |
| MOTA | 1140 | 0 | | | 39.495 | 3.941 | 117.178 | 1.00 16.63 |
| ATOM | 1141 | N | ASN A 146 | | 39.423 | 4 160 | 118.628 | 1.00 23.57 |
| MOTA | 1142 | CA | ASN A 146 | | 40.708 | | | 1.00 19.80 |
| ATOM | 1143 | CB | ASN A 146 | | | | 118.967 | 1.00 27.81 |
| ATOM | 1144 | CG | ASN A 146 | | 41.924 | | | 1.00 19.55 |
| ATOM | 1145 | OD1 | ASN A 146 | | 42.299 | 5.421 | 119.704 | 1.00 19.55 |
| ATOM | 1146 | ND2 | ASN A 146 | | 42.544 | 4.202 | 117.827 | |
| ATOM | 1147 | C | ASN A 146 | | 39.079 | | 119.023 | 1.00 26.32 |
| | 1148 | ō | ASN A 146 | | 38.452 | 5.827 | 120.059 | 1.00 28.34 |
| ATOM | | N | PRO A 147 | | 39.512 | 6.605 | 118.231 | 1.00 28.46 |
| ATOM | 1149 | | PRO A 147 | | 40.383 | 6.637 | 117.042 | 1.00 27.18 |
| ATOM | 1150 | CD | PRO A 147 | | 39.150 | 7.972 | 118.618 | 1.00 24.15 |
| MOTA | 1151 | CA | | | 39.859 | | 117.558 | 1.00 25.13 |
| MOTA | 1152 | CB | PRO A 147 | | 41.081 | | 117.235 | 1.00 30.05 |
| ATOM | 1153 | CG | PRO A 147 | | 37.618 | 9 136 | 118.578 | 1.00 26.71 |
| ATOM | 1154 | С | PRO A 147 | | | | 119.456 | 1.00 24.93 |
| ATOM | 1155 | 0 | PRO A 147 | | 37.017 | 7.557 | 117.562 | 1.00 21.42 |
| MOTA | 1156 | N | ALA A 148 | | 36.989 | 7.557 | 117.302 | 1.00 21.03 |
| MCTA | 1157 | CA | ALA A 148 | | 35.536 | | 117.416 | 1.00 19.98 |
| ATOM | 1158 | CB | ALA A 148 | | 35.112 | 7.044 | 116.072 | 1.00 20.40 |
| ATOM | 1159 | c | ALA A 148 | | 34.838 | 6.891 | . 118.552 | 1.00 20.49 |
| | 1160 | Ö | ALA A 148 | | 33.822 | 7.344 | 119.067 | 1.00 21.44 |
| ATOM | 1161 | N | VAL A 149 | | 35.381 | 5.739 | 118.928 | 1.00 19.20 |
| ATOM | | CA | VAL A 149 | | 34.818 | 4.950 | 120.016 | 1.00 24.61 |
| MOTA | 1162 | | VAL A 149 | | 35.570 | 3.608 | 120.181 | 1.00 25.96 |
| MOTA | 1163 | CE | | | 35.158 | 2.918 | 3 121.485 | 1.00 26.58 |
| ATOM | 1164 | CG. | 1 VAL A 149 | | 35.262 | 2.704 | 118.995 | 1.00 25.67 |
| ATOM | 1165 | | 2 VAL A 149 | | 34.947 | 5.752 | 2 121.304 | 1.00 23.56 |
| ATOM | 1166 | С | VAL A 149 | | 33.990 | 5 88 | 7 122.064 | 1.00 22.52 |
| MOTA | 1167 | 0 | VAL A 149 | | | 6 28 | 7 121.536 | 1.00 24.65 |
| ATOM | 1168 | N | GLY A 150 | | 36.143 | 7 07 | 122.731 | 1.00 22.82 |
| ATOM | 1169 | CA | | | 36.390 | 7.07 | 1 122.838 | 1.00 25.46 |
| ATOM | 1170 | С | GLY A 150 | | 35.477 | 8.26. | 1 122.030 | 1.00 23.17 |
| ATOM | 1171 | 0 | GLY A 150 | | 34.919 | 8.564 | 4 123.904 | 1.00 24.38 |
| ATOM | 1172 | N | ILE A 151 | | 35.327 | 9.00 | 1 121.733 | |
| | 1173 | CA | | | 34.481 | 10.18 | 0 121.716 | 1.00 22.65 |
| ATOM | 1174 | CB | | | 34.610 | 10.92 | 8 120.371 | 1.00 24.45 |
| ATOM | | | | | 33.598 | 12.07 | 7 120.306 | 1.00 24.71 |
| ATOM | 1175 | | 2 ILE A 131 | | 36.041 | 11.46 | 2 120.222 | 1.00 28.02 |
| ATOM | 1176 | | | | 36.354 | | 6 118.854 | 1.00 27.10 |
| ATOM | 1177 | | 1 ILE A 151 | | 33.018 | | 6 121.987 | 1.00 28.19 |
| ATOM | 1178 | | ILE A 151 | | 32.337 | _ | 2 122.763 | |
| ATOM | 1179 | | ILE A 151 | | | | 4 121.364 | |
| ATOM | 1180 | N | GLU A 152 | | 32.532 | | 4 121.601 | |
| ATOM | 1181 | | GLU A 152 | | 31.149 | | 1 120.672 | |
| ATOM | 1182 | | GLU A 152 | | 30.758 | | 1 120.072 | |
| ATOM | 1183 | | GLU A 152 | | 30.609 | | 3 119.194 | |
| | 1184 | | 4 - 6 | | 29.455 | | 4 118.946 | |
| ATOM | 1185 | | | | 29.139 | | 7 117.773 | |
| ATOM | 1186 | | 150 | | 28.862 | | | |
| ATOM | | | GLU A 152 | | 31.009 | 7.87 | 9 123.055 | 1.00 28.00 |
| ATCM | 1187 | | GLU A 152 | | 29.980 | 8.09 | 6 123.683 | 1.00 31.23 |
| RIOM | 1188 | 3 0 | GDO A 102 | | = - | | | |
| | | | | | | | | |

| | | | | • | | | |
|--------|-------|-----|-------------|---|--------|----------------|------------|
| 3 TOM | 1189 | N | TYR A 153 | | 32.054 | 7.253 123.583 | 1.00 28.72 |
| MOTA | | | TYR A 153 | | 32.066 | 6.805 124.971 | 1.00 31.35 |
| MOTA | 1190 | CA | | | 33.427 | 6.204 125.307 | 1.00 31.56 |
| MOTA | 1191 | CB | TYR A 153 | | | | 1.00 33.17 |
| ATOM | 1192 | CG | TYR A 153 | | 33.617 | | |
| ATOM | 1193 | CD1 | TYR A 153 | | 33.111 | 4.647 127.280 | 1.00 35.43 |
| | | CE1 | TYR A 153 | | 33.321 | 4.298 128.619 | 1.00 33.52 |
| ATOM | 1194 | | | | 34.329 | 6.677 127.611 | 1.00 34.29 |
| MOTA | 1195 | CD2 | TYR A 153 | | | • • • • • | 1.00 35.34 |
| ATOM | 1196 | CE2 | TYR A 153 | | 34.544 | | |
| ATOM | 1197 | CZ | TYR A 153 | | 34.041 | 5.154 129.444 | |
| | 1198 | OH | TYR A 153 | • | 34.260 | 4.835 130.767 | 1.00 30.10 |
| MOTA | | | TYR A 153 | | 31.828 | 8.022 125.857 | 1.00 32.71 |
| MOTA | 1199 | С | | | | 7.988 126.787 | 1.00 29.14 |
| ATOM | 1200 | 0 | TYR A 153 | | 31.026 | | 1.00 29.65 |
| MOTA | 1201 | N | LEU A 154 | | 32.538 | | |
| ATOM | 1202 | CA | LEU A 154 | | 32.413 | 10.332 126.310 | 1.00 32.87 |
| | 1203 | СВ | LEU A 154 | | 33.477 | 11.329 125.847 | 1.00 31.46 |
| MOTA | | | LEU A 154 | | 34.910 | 11.053 126.324 | 1.00 29.68 |
| MOTA | 1204 | CG. | LEU A 154 | | 35.898 | 11.953 125.605 | 1.00 29.29 |
| MOTA | 1205 | CD1 | | | | 11.278 127.829 | 1.00 27.19 |
| ATOM | 1206 | CD2 | | | 34.989 | | 1.00 34.63 |
| ATOM | 1207 | С | LEU A 154 | | 31.020 | | |
| ATOM | 1208 | 0 | LEU A 154 | | 30.475 | 11.379 127.250 | 1.00 32.58 |
| | | N | ARG A 155 | | 30.443 | 10.999 125.035 | 1.00 36.63 |
| MOTA | 1209 | | | | 29.107 | 11.569 124.869 | 1.00 38.36 |
| ATOM | 1210 | CA | ARG A 155 | | | 11.502 123.405 | 1.00 36.32 |
| ATOM | 1211 | CB | ARG A 155 | | 28.661 | | 1.00 43.15 |
| ATOM | 1212 | CG | ARG A 155 | | 29.581 | 12.253 122.460 | |
| ATOM | 1213 | CD | ARG A 155 | | 29.100 | 12.201 121.023 | 1.00 41.10 |
| | 1214 | NE | ARG A 155 | | 27.936 | 13.047 120.768 | 1.00 44.00 |
| MOTA | | | ARG A 155 | | 27.331 | 13.140 119.583 | 1.00 54.07 |
| ATOM | 1215 | CZ | ARG A 155 | | 27.772 | 12.441 118.540 | 1.00 51.61 |
| MOTA | 1216 | NH1 | | • | | 13.948 119.424 | 1.00 51.76 |
| MOTA | 1217 | NH2 | | | 26.291 | | 1.00 36.25 |
| ATOM | 1218 | C | ARG A 155 | | 28.112 | 10.821 125.745 | |
| ATOM | 1219 | 0 | ARG A 155 | | 27.270 | 11.433 126.397 | 1.00 39.00 |
| | 1220 | N | LYS A 156 | | 28.213 | 9.496 125.765 | 1.00 36.48 |
| MOTA | | | LYS A 156 | | 27.315 | 8.698 126.587 | 1.00 39.06 |
| MOTA | 1221 | CA | | | 27.460 | 7.213 126.256 | 1.00 41.88 |
| MOTA | 1222 | CB | LYS A 156 | | 26.672 | 6.816 125.020 | 1.00 51.15 |
| ATOM | 1223 | CG | LYS A 156 | | | 7.505 123.781 | 1.00 55.56 |
| MOTA | 1224 | CD | LYS A 156 | | 27.169 | | 1.00 55.63 |
| ATOM | 1225 | CE | LYS A 156 | | 26.117 | 7.502 122.676 | |
| ATOM | 1226 | NZ | LYS A 156 | | 24.993 | 8.425 123.013 | 1.00 49.15 |
| | 1227 | C | LYS A 156 | | 27.527 | 8.932 128.076 | 1.00 39.91 |
| ATOM | | | LYS A 156 | | 26.636 | 8.658 128.876 | 1.00 37.01 |
| MOTA | .1228 | 0 | | | 28.703 | 9.431 128.448 | 1.00 37.73 |
| MOTA | 1229 | N | LYS A 157 | | 28.985 | 9.725 129.847 | 1.00 36.52 |
| MOTA | 1230 | CA | LYS A 157 | | | 9.700 130.122 | 1.00 35.64 |
| MOTA | 1231 | CB | LYS A 157 | | 30.493 | 9.700 130.122 | 1.00 35.44 |
| MOTA | 1232 | CG | LYS A 157 | | 31.094 | 8.308 130.174 | 1.00 33.44 |
| | 1233 | CD | LYS A 157 | | 30.509 | 7.510 131.335 | 1.00 31.28 |
| MOTA | | CE | LYS A 157 | | 31.077 | 6.106 131.388 | 1.00 31.48 |
| ATOM | 1234 | | 113 A 137 | | 30.464 | 5.310 132.493 | 1.00 36.39 |
| MOTA | 1235 | NZ | LYS A 157 | | 28.423 | 11.097 130.197 | |
| ATOM | 1236 | C | LYS A 157 | | | 11.547 131.336 | |
| ATOM | 1237 | 0 | LYS A 157 | | 28.531 | TI.34/ T31.330 | |
| ATOM | 1238 | N | GLY A 158 | | 27.842 | 11.768 129.205 | |
| | 1239 | CA | GLY A 158 | | 27.257 | 13.074 129.452 | 1.00 34.31 |
| MOTA | | | GLY A 158 | | 27.972 | 14.293 128.894 | 1.00 36.36 |
| ATOM | 1240 | C | | | 27.438 | 15.399 128.963 | 1.00 32.96 |
| ATOM | 1241 | 0 | GLY A 158 | | | 14.117 128.344 | |
| ATOM | 1242 | N | PHE A 159 | | 29.170 | 15 250 127 705 | |
| ATOM | 1243 | CA | PHE A 159 | | 29.892 | 15.260 127.796 | |
| | 1244 | CB | PHE A 159 | | 31.346 | 14.892 127.504 | 1.00 28.62 |
| ATOM | | CG | PHE A 159 | | 32.137 | 14.555 128.730 | 1.00 28.80 |
| MOTA | 1245 | | | | 32.043 | 13.300 129.310 | 1.00 30.41 |
| MOTA | 1246 | CD: | 1 PHE A 159 | | 32.951 | 15.513 129.327 | |
| ATOM | 1247 | ÇD: | | | | 12.996 130.472 | |
| ATOM | 1248 | CE: | 1 PHE A 159 | | 32.749 | | |
| | 1249 | CE | | | 33.661 | 15.223 130.488 | |
| MOTA | 1250 | | PHE A 159 | | 33.561 | 13.963 131.062 | 1.00 32.32 |
| ATOM | | | PHE A 159 | | 29.224 | 15.786 126.536 | 1.00 28.88 |
| ATOM | 1251 | C | PUD A 107 | | 28.765 | | 1.00 27./1 |
| ATOM | 1252 | 0 | PHE A 159 | | | 100 400 | |
| · ATCM | 1253 | N | LYS A 160 | | 29.180 | | |
| MOTA | 1254 | | LYS A 160 | | 28.550 | 17.766 125.25 | 1.00 33.30 |

| | | | | | _ | | | | |
|--------------|--------------|----------|------------------|------------|------------------|------------------|---------------------------------------|--------|------------------|
| ATOM | 1255 | CB L | 'S A 1 | 60 | 27.390 | | 125.719 | 1.00 3 | |
| MOTA | 1256 | | is A 1 | 60 | 26.273 | | 126.419 | 1.00 3 | |
| MOTA | 1257 | | 'S A 1 | | 25.105 | | 126.723 127.651 | 1.00 5 | |
| MOTA | 1258 | | YS A 1 | | 25.500 | | 129.008 | 1.00 4 | |
| MOTA | 1259 | | YS A 1 | | 25.924 | _, | 124.394 | 1.00 | |
| MOTA | 1260 | C L | /S A 1 | .60 | 29.484 29.093 | | 123.327 | | 30.98 |
| MOTA | 1261 | 0 17 | YS A 1 | .60 | 30.700 | | 124.867 | | 31.43 |
| MOTA | 1262 | | RG A 1 | | 31.665 | | 124.108 | 1.00 2 | |
| ATOM | 1263 | | RG A 1 | | 31.781 | 21.048 | 124.673 | | 34.45 |
| ATOM | 1264 1265 | | RG A 1 | | 30.476 | 21.854 | 124.610 | 1.00 | |
| MOTA MOTA | 1266 | | RG A 1 | | 30.705 | | 124.966 | | 39.01 |
| ATOM | 1267 | | RG A 1 | | 31.158 | | 126.341 | 1.00 | |
| ATOM | 1268 | CZ A | RG A 1 | 61 | 30.389 | | 127.414 | _ | 43.33 · 45.95 |
| MOTA | 1269 | NH1 A | RG A 1 | 161 | 29.117 | | 127.274 128.627 | | 43.74 |
| MOTA | 1270 | NH2 A | RG A 1 | 61 | 30.893 | | 128.027 | | 32.71 |
| ATOM | 1271 | | RG A 1 | | 33.009 33.792 | | 125.092 | | 28.53 |
| MOTA | 1272 | | RG A 1 | | 33.752 | | 123.149 | | 32.50 |
| MOTA | 1273 | | LE A 1 LE A 1 | | 34.485 | | 123.049 | | 28.52 |
| MOTA | 1274 | | LE A | | 34.146 | 15.821 | 122.820 | | 31.42 |
| ATOM | 1275 1276 | | LE A | | 35.407 | 14.976 | 122.898 | | 24.95 |
| ATOM ATOM | 1277 | | LE A | | 33.147 | | 123.879 | | 30.25 |
| ATOM | 1278 | | LE A | | 32.564 | 13.977 | | | 34.27 |
| ATOM | 1279 | c I | LE A | 162 | 35.353 | 17.816 | 121.886 | | 26.46 27.88 |
| ATOM | 1280 | 0 [| LE A | 162 | 34.876 | 17.973 18.067 | 120.762 122.168 | | 23.13 |
| ATOM | 1281 | N _ | EU A | 163 | 36.626 37.575 | 18.534 | | 1.00 | 25.74 |
| MOTA | 1282 | | EU A | | 38.384 | 19.729 | 121.681 | | 26.25 |
| MOTA | 1283 | | A UE. A UE. | | 39.626 | 20.138 | 120.862 | 1.00 | 24.39 |
| ATOM | 1284 1285 | | EU A | | 39.213 | 20.591 | 119.473 | | 26.25 |
| MOTA MOTA | 1285 | CD2 L | EU A | 163 | 40.361 | | 121.560 | | 27.76 |
| MOTA | 1287 | | EU A | | 38.547 | 17.416 | | | 27.09 |
| ATOM | 1288 | 0 L | EU A | 163 | 39.053. | 16.721 | | | 25.25 26.97 |
| ATOM | 1289 | | YR A | | 38.808 | 17.257 16.241 | | 1 00 | 26.97 |
| MOTA | 1290 | | YR A | | 39.747 39.021 | 15.181 | | 1.00 | 23.38 |
| MOTA | 1291 | | TYR A | | 39.944 | | 117.565 | 1.00 | 21.76 |
| ATOM | 1292 | | TYR A | | 40.563 | 13.179 | 118.353 | 1.00 | 22.49 |
| ATOM | 1293 1294 | | YR A | | 41.419 | 12.224 | 117.794 | | 22.90 |
| MOTA MOTA | 1295 | | YR A | | 40.202 | 14.142 | | 1.00 | 18.74 |
| ATOM | 1296 | CE2 | TYR A | 164 | 41.060 | 13.190 | | 1.00 | 23.36 21.50 |
| ATOM | 1297 | | TYR A | | 41.663 | 12.235 | 116.426 | 1.00 | 18.41 |
| ATOM | 1298 | | TYR A | | 42.506 40.798 | 16.923 | | | 21.67 |
| ATOM | 1299 | C | TYR A | 164 | 40.73 | 17 511 | 117.112 | | 19.75 |
| MOTA | 1300 | 0 7 | TYR A | 165 | 42.057 | 16.843 | 118.551 | 1.00 | 25.61 |
| MOTA | 1301 1302 | N : | LLE A | 165 | 43.149 | 17.462 | 117.804 | 1.00 | 24.43 |
| MOTA MOTA | 1302 | | LE A | | 43.963 | 18.396 | 118.717 | | 26.41 |
| MOTA | 1304 | CG2 | LE A | 165 | 45.127 | 19.017 | 117.937 | | 19.36 23.36 |
| ATOM | 1305 | CG1 | ILE A | 165 | 43.035 | 19.482 | | | 25.05 |
| ATOM | 1306 | CD1 | ILE A | 165 | 43.685 | 20.402 16.36 | | 1 00 | 26.91 |
| MOTA | 1307 | | ILE A | | 44.040 44.538 | 15.50 | · · · · · · · · · · · · · · · · · · · | 1.00 | 21.91 |
| MOTA | 1308 | 0 | ILE A | 165 | 44.242 | 16.40 | | 1.00 | 24.20 |
| MOTA | 1309 | N I | ASP A | 166 | 45.022 | 15.38 | | 1.00 | 27.11 |
| ATOM | 1310 | AC EC | ASP A | 166 | 44.140 | 14.76 | 5 114.137 | 1.00 | 28.56 |
| ATOM | 1311 1312 | CS . | ASP A | 166 | 44.699 | 13.46 | 1 113.599 | | 34.59 |
| atom atom | 1313 | OD1 | ASP A | 166 | 45.831 | 13.45 | | | 30.37 |
| ATOM | 1314 | OD2 | ASP A | 166 | 43.995 | 12.43 | 7 113.717 | | 23.27 24.47 |
| ATOM | 1315 | С. | ASP A | 166 | 46.319 | 15.92 | | | 23.19 |
| ATCM | 1316 | o. | ASP A | 166 | 46.295 | 16.61 | | | 23.43 |
| ATOM | 1317 | | LEU A | 167 | 47.452 48.738 | 15.59 16.06 | | 1.00 | 24.67 |
| ATOM | 1318 | CA | LEU A | 10/ 167 | 49.682 | | | 1.00 | 21.90 |
| ATOM | 1319 | | LEU A | 167 | 49.002 | 17.44 | | | 26.62 |
| ATOM | 1320 | CG | LEU A | 107 | 47.240 | _ , | | | |

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 1321 1322 1323 1324 1325 1326 1327 1329 1333 1333 1333 1333 1333 1334 1343 1344 1345 1346 1347 1348 1349 1351 1353 1355 1355 1355 1355 1355 135 | CD1 LEU A 167 CD2 LEU A 167 C LEU A 167 C LEU A 167 N ASP A 168 CA ASP A 168 CB ASP A 168 CG ASP A 168 C ASP A 168 O ASP A 168 OD1 ASP A 168 OD2 ASP A 168 OD2 ASP A 168 N ALA A 169 CA ALA A 169 CA ALA A 169 C ALA A 169 C ALA A 169 C HIS A 170 C HIS A 170 C HIS A 170 C HIS A 170 CHIS A 170 CD2 HIS A 170 CD2 HIS A 170 CD2 HIS A 170 CD2 HIS A 171 CD3 HIS A 171 CB HIS A 171 CD HIS A 171 CHIS A 171 | 50.249 48.658 49.405 50.504 48.736 49.244 48.209 48.722 49.423 48.629 48.777 50.448 50.693 52.068 49.612 49.643 47.554 46.04 47.55 48.83 49.84 50.82 50.50 45.31 43.99 43.23 41.83 40.72 39.66 43.16 43.46 | 18.668 15.092 15.345 13.977 12.975 11.852 10.669 13.686 14.559 9.644 10.750 13.3127 13.927 13.498 13.498 14.204 12.746 12.445 12.867 12.867 12.849 10.950 10.420 9.982 9.634 10.329 9.828 13.661 14.719 31.661 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 91.648 14.779 31.669 | 116.092 113.755 113.262 113.488 112.555 112.410 111.608 111.209 110.865 112.227 110.364 109.140 108.601 108.601 108.601 107.468 109.255 107.311 106.570 107.385 107.385 107.385 107.131 106.570 107.591 106.746 107.634 106.766 107.634 106.766 | 1.00 25.88 1.00 22.40 1.00 25.82 1.00 21.89 1.00 24.59 1.00 27.12 1.00 28.11 1.00 24.17 1.00 17.18 1.00 25.40 1.00 25.40 1.00 25.40 1.00 25.40 1.00 26.57 1.00 26.57 1.00 26.57 1.00 26.57 1.00 24.79 1.00 24.12 1.00 24.13 1.00 24.13 1.00 24.13 1.00 24.33 1.00 24.33 1.00 24.33 1.00 22.88 1.00 21.89 1.00 21.14 1.00 25.57 1.00 25.57 1.00 25.57 1.00 25.57 1.00 25.57 1.00 25.57 1.00 25.57 1.00 25.55 1.00 25.35 1.00 29.61 1.00 27.62 1.00 27.62 1.00 26.52 |
|---|---|---|--|---|--|--|
| MOTA MOTA | 1358 1359 | N CYS A 172 CA CYS A 172 | 41.61 41.46 | | 109.987 111.456 | 1.00 24.82. 1.00 29.47 |
| MOTA | 1360 1361 | CB CYS A 172 SG CYS A 172 | 40.95 | 9 14.065 | 111.717 | 1.00 25.69 |
| ATOM ATOM | 1362 | C CYS A 172 | 40.23 | 7 11.797 | 109.314 | 1.00 28.21 1.00 26.78 |
| ATOM | 1363 | O CYS A 172 | 39.21 40.23 | | | 1.00 22.05 |
| ATOM | 1364 1365 | N ASP A 173 CA ASP A 173 | 38.94 | 9 11.217 | 107.350 | 1.00 27.39 |
| MOTA MOTA | 1366 | CB ASP A 173 | 39.10 | | 105.931 105.922 | 1.00 30.47 1.00 29.77 |
| ATOM | 1367 | CG ASP A 173 OD1 ASP A 173 | 39.82 39.88 | 8.658 | 3 104.830 | 1.00 21.14 |
| MOTA MOTA | 1368 1369 | OD2 ASP A 173 | 40.2 | 38 8.787 | 7 106.978 | 1.00 30.04 1.00 27.86 |
| ATOM | 1370 | C ASP A 173 | 37.8 | | 108.105 2 108.120 | |
| MOTA | 1371 | | 36.7 38.3 | | 5 108.753 | 1.00 25.84 |
| ATOM | 1372 | | 37.3 | 44 8.513 | 3 109.490 | 1.00 28.49 |
| MOTA MOTA | 1373 1374 | | 36.6 | 94 9.29 | 6 110.619 | 1.00 26.14 1.00 21.39 |
| ATOM | 1375 | O GLY A 174 | 35.4 | | 7 110.780 4 111.409 | |
| ATOM | 1376 | | 37.5 36.9 | | | 1.00 25.53 |
| MOTA | 1377 | | 38.1 | | 9 113.401 | 1.00 30.54 |
| ATOM | 1378 1379 | | 37.5 | 65 12.10 | 5 114.566 | 1.00 28.02 |
| ATOM ATOM | 1380 | CG2 VAL A 175 | 38.9 | 73 10.12 | | |
| ATOM | 1381 | C VAL A 175 | 36.1 | 63 11.95 30 12.28 | | 1.00 21.60 |
| ATCM | 1382 | 0 VAL A 175 | 35.1 36.6 | | | 1.00 25.43 |
| ATOM | 1383 | | | 54 13.73 | 0 110.426 | 1.00 26.12 |
| ATOM | 1384 1385 | 17/ | 36.5 | 54 14.33 | 6 109.205 | 1.00 24.71 |
| ATCM ATOM | | | | | 9 108.469 | 1.00 20.00 |

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| - ምርነፈ | 1387 | CD GLN A 176 | | 36.385 | 16.002 107.30 | 6 1.00 29.54 |
| atom Atom | 1388 | OE1 GLN A 176 | | 37.382 | 16.704 107.48 | 6 1.00 26.93 |
| ATOM | 1389 | NE2 GLN A 176 | | 35.872 | 15.776 106.09 | 9 1.00 27.58 9 1.00 27.63 |
| ATCM | 1390 | C GLN A 176 | | 34.446 | 13.316 110.02 | |
| ATOM | 1391 | O GLN A 176 | | 33.481 | 14.021 110.31 | |
| ATOM | 1392 | N GLU A 177 | | 34.330 | 12.173 109.36 | |
| MOTA | 1393 | CA GLU A 177 | | 33.027 | 11.696 108.91 10.445 108.05 | 3 1.00 34.20 |
| MOTA | 1394 | CB GLU A 177 | | 33.181 | 10.069 107.32 | |
| MOTA | 1395 | CG GLU A 177 | | 31.905 | 8.819 106.49 | |
| ATOM | 1396 | CD GLU A 177 | | 32.060 32.056 | 7.712 107.07 | |
| MOTA | 1397 | OE1 GLU A 177 | | 32.206 | 8.947 105.26 | |
| MOTA | 1398 | OE2 GLU A 177 C GLU A 177 | | 32.128 | 11.377 110.09 | 99 1.00 30.54 |
| MOTA | 1399 | | | 30.945 | 11.697 110.09 | 93 1.00 25.39 |
| MOTA | 1400 | | | 32.707 | 10.750 111.13 | 14 1.00 27.03 |
| MOTA | 1401 1402 | N ALA A 178 CA ALA A 178 | | 31.971 | 10.365 112.30 | 03 1.00 30.67 |
| ATOM | 1402 | CB ALA A 178 | | 32.905 | 9.658 113.2 | 89 1.00 30.49 |
| MOTA MOTA | 1404 | C ALA A 178 | | 31.261 | 11.519 113.0 | 03 1.00 33.21 |
| ATOM | 1405 | O ALA A 178 | | 30.145 | 11.355 113.4 | |
| ATOM | 1406 | N PHE A 179 | | 31.888 | 12.688 113.0 | |
| ATOM | 1407 | CA PHE A 179 | | 31.256 | 13.801 113.7 14.128 115.0 | |
| ATCM | 1408 | CB PHE A 179 | | 32.071 | 12.909 115.7 | |
| ATOM | 1409 | CG PHE A 179 | | 32.469 | 12.375 115.6 | |
| ATOM | 1410 | CD1 PHE A 179 | | 33.749 31.536 | 12.233 116.5 | |
| MOTA | 1411 | CD2 PHE A 179 | | 34.103 | 11.184 116.2 | 93 1.00 16.56 |
| ATOM | 1412 | CE1 PHE A 179 CE2 PHE A 179 | | 31.881 | 11.038 117.2 | 04 1.00 26.38 |
| MOTA | 1413 | CE2 PHE A 179 CZ PHE A 179 | | 33.170 | 10.515 117.0 | 67 1.00 20.30 |
| MOTA | 1414 1415 | C PHE A 179 | | 31.079 | 15.037 112.8 | |
| MOTA | 1416 | O PHE A 179 | | 31.006 | 16.152 113.3 | |
| MOTA MOTA | 1417 | N TYR A 180 | | 30.980 | 14.828 111.5 | 384 1.00 31.68 346 1.00 32.76 |
| ATOM | 1418 | CA TYR A 180 | | 30.829 | 15.925 110.6 | |
| ATOM | 1419 | CB TYR A 180 | | 30.931 | 15.378 109.2 16.406 108.3 | |
| ATOM | 1420 | CG TYR A 180 | | 31.331 | 16.846 107.2 | |
| MOTA | 1421 | CD1 TYR A 180 | | 30.427 30.801 | 17.791 106.2 | |
| ATOM | 1422 | CE1 TYR A 180 | | 32.624 | 16.937 108.3 | 1.00 36.32 |
| MOTA | 1423 | CD2 TYR A 180 CE2 TYR A 180 | | 33.007 | 17.879 107.2 | 203 1.00 37.83 |
| MOTA | 1424 | | | 32.088 | 18.304 106.2 | 250 1.00 36.05 |
| ATOM | 1425 1426 | OH TYR A 180 | | 32.446 | 19.255 105.3 | 323 1.00 28.04 |
| ATOM | 1427 | C TYR A 180 | | 29.518 | 16.696 110.8 | 825 1.00 30.94 |
| ATOM ATOM | 1428 | O TYR A 180 | | 29.459 | 17.894 110. | 560 1.00 30.42 299 1.00 31.56 |
| ATOM | 1429 | N ASP A 181 | | 28.473 | 16.026 111.1 16.691 111. | |
| ATOM | 1430 | CA ASP A 181 | | 27.180 | 16.691 111. 15.833 110. | |
| ATOM | 1431 | CB ASP A 181 | | 26.086 | 14.689 111. | |
| ATOM | 1432 | CG ASP A 181 | | 25.645 26.505 | 13.963 112. | |
| ATOM | 1433 | OD1 ASP A 181 | | 24.425 | 14.504 111. | 871 1.00 46.56 |
| ATOM | 1434 | OD2 ASP A 181 | | 26.754 | 17.044 112. | 866 1.00 36.81 |
| ATOM | 1435 | C ASP A 181 O ASP A 181 | | 25.571 | 17.286 113. | 109 1.00 33.91 |
| ATCM | 1436 1437 | O ASP A 181 N THR A 182 | | 27.689 | 17.066 113. | 810 1.00 40.86 |
| ATOM | 1437 | CA THR A 182 | | 27.327 | 17.412 115. | 184 1.00 38.27 |
| ATOM ATOM | 1439 | | | 27.433 | 16.201 116. | 133 1.00 37.99 |
| ATOM | 1440 | | | 27.013 | 16.595 117. | 448 1.00 35.64 194 1.00 35.61 |
| ATOM | 1441 | | | 28.869 | | |
| ATOM | 1442 | C THR A 182 | | 28.177 | | |
| ATOM | 1443 | O THR A 182 | | 29.365 | | |
| ATOM | 1444 | N ASP A 183 | | 27.557 | | |
| ATCM- | 1445 | CA ASP A 183 | | 28.250 27.313 | | 228 1.00 35.56 |
| ATOM | 1446 | | • | 26.136 | | 155 1.00 38.01 |
| ATOM | 1447 | CG ASP A 183 | | 25.614 | 20,357 118. | .210 1.00 34.94 |
| MOTA | 1448 | OD1 ASP A 183 | | 25.720 | 22,470,118 | .814 1.00 38.1/ |
| atom | 1449 | | | 28.762 | 20 161 118 | .578 1.00 35.27 |
| ATCM | 1450 | | | 29.337 | 21.015 119 | .251 1.00 35.16 |
| ATCM | 1451 1452 | | | 28.562 | | .012 1.00 35.10 |
| ATOM | 1494 | v GLIV A 104 | | | | |

| | • | |
|--------------|--|--|
| | 1453 CA GLN A 184 | 29.030 18.505 120.333 1.00 35.16 |
| MOTA | 104 | 28 155 17.382 120.906 1.00 36.94 |
| MOTA | 104 | 26.663 17.718 120.988 1.00 38.34 |
| MOTA | | 25 881 16,725 121.838 1.00 43.68 |
| ATOM | | 26 027 15,512 121.696 1.00 35.48 |
| MOTA | | 25 036 17 243 122 723 1.00 51.06 |
| ATOM | 101 | 30 479 18.035 120.253 1.00 36.32 |
| MOTA | 104 | 31 135 17.825 121.275 1.00 34.24 |
| ATOM | 105 | 30 976 17.883 119.028 1.00 34.51 |
| ATOM | 105 | 32 348 17.443 118.804 1.00 33.59 |
| ATOM | 105 | 32 393 15,990 118.259 1.00 33.11 |
| MOTA | | 33 834 15.567 118.003 1.00 23.80 |
| ATOM | 1464 CG1 VAL A 185 1465 CG2 VAL A 185 | 31 731 15.045 119.242 1.00 26.00 |
| MOTA | | 33.053 18.354 117.803 1.00 33.11 |
| MOTA | 105 | 32 545 18.593 116.714 1.00 27.73 |
| MOTA | | 34 215 18.872 118.184 1.00 31.49 |
| MOTA | 106 | 34 985 19.729 117.291 1.00 30.03 |
| MOTA | 106 | 35 420 21.023 117.991 1.00 30.34 |
| MOTA | | 36 008 22.047 117.051 1.00 30.22 |
| MOTA | - 100 | 35 265 23,156 116.656 1.00 32.23 |
| MOTA | 106 | 37 284 21.879 116.524 1.00 29.37 |
| MOTA | 106 | 35 785 24.078 115.748 1.00 27.07 |
| MOTA | 106 | 37 813 22 794 115 615 1.00 28 54 |
| ATOM | | 37 064 23.892 115.227 1.00 30.00 |
| MOTA | 106 | 36.232 18.952 116.879 1.00 33.38 |
| MOTA | - non n 106 | 36.952 18.426 117.729 1.00 28.30 |
| MOTA | 107 | 36.478 18.877 115.574 1.00 32.00 |
| MOTA | 107 | 37.645 18.171 115.060 1.00 29.70 37.252 17.095 114.019 1.00 30.03 |
| MOTA | 1480 CA VAL A 187 1481 CB VAL A 187 | 37.232 17.033 22 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |
| MOTA | 1482 CG1 VAL A 187 | |
| MOTA | 1483 CG2 VAL A 187 | 30.410 10.003 100 1 00 31 03 |
| MOTA | 1484 C VAL A 187 | 30.004 13.135 147 1 00 31 88 |
| ATOM ATOM | 1485 O VAL A 187 | 38.213 13.00 24 88 |
| MOTA | 1486 N LEU A 188 | 39.030 13.131 14.204 1.00.26.92 |
| MOTA | 1487 CA LEU A 188 | 40.033 20.010 10.00 27 04 |
| ATOM | 1488 CB LEU A 188 | 41.400 20.555 1.00 25 15 |
| MOTA | 1489 CG LEU A 188 | 42.023 22.333 143 649 1 00 18 53 |
| ATOM | 1490 CD1 LEU A 188 | 42.000 22.333 116 060 1 00 28 81 |
| MOTA | 1491 CD2 LEU A 188 | 43.330 22.403 22.403 23.33 |
| ATOM | 1492 C LEU A 188 | 42.022 13.113 114 507 1 00 25 83 |
| ATOM | 1493 O LEU A 188 | 42.373 10.333 1.00 30 53 |
| ATOM | 1294 N SER A 189 | 42.303 13.20 007 1 00 30 13 |
| ATOM | 1495 CA SER A 189 | 43.423 10.33 43 |
| ATCM | :496 CB SER A 189 | 12.021 16.474 110 588 1.00 32.98 |
| MOTA | 1497 OG SER A 189 | 43.837 10.170 111 143 1.00 27.94 |
| ATOM | 1498 C SER A 189 | 14 004 10 891 11 253 1.00 22.14 |
| ATOM | 1499 O SER A 189 | 4E 720 19 877 11 423 1.00 24.60 |
| ATOM | 1500 N LEU A 190 | 46 805 19 438 110.614 1.00 22.23 |
| MOTA | 1501 CA LEU A 190 | 47 055 20 000 111 459 1.00 23.69 |
| ATCM | 1502 CB LEU A 190 | 47 722 21 075 112 522 1.00 28.94 |
| MOTA | 1503 CG LEU A 190 | 10 070 21 780 112 740 1.00 43.01 |
| ATOM | 1504 CD1 LEU A 190 | 16 CO1 22 OQ3 112 OB7 1.00 28 II |
| MOTA | 1505 CD2 LEU A 190 | 10 200 10 210 109 872 1.00 44.09 |
| MOTA | 1506 C LEU A 190 | - 416 17 141 110 465 1.00 10.33 |
| MOTA | 1507 O LEU A 190 | 47 599 18.353 108.587 1.00 19.22 |
| MOTA | 1508 N HIS A 191 | 48 046 17.210 107.804 1.00 23.28 |
| MOTA | 1509 CA HIS A 191 | 16 870 16 242 107 650 1.00 13.30 |
| ATOM | 1510 CB HIS A 191 | 45 591 16.915 107.256 1.00 24.16 |
| ATOM | 1511 CG HIS A 191 | 15 034 17.124 106.038 1.00 17.71 |
| ATOM | 1512 CD2 HIS A 191 | 44 595 17,419 108.176 1.00 23.76 |
| ATOM | 1513 ND1 HIS A 191 | 43 644 17.913 107.545 1.00 19.70 |
| ATOM | 1514 CE1 HIS A 191 | 43 823 17 746 106.246 1.00 27.67 |
| ATCM | | 49 570 17 620 106.434 1.00 23.63 |
| ATOM | 727 101 | 40 419 18 761 106.017 1.00 23.03 |
| ATOM | | 48.419 18.761 1001017 49.209 16.681 105.746 1.00 23.49 |
| ATOM | 1518 N GLN A 192 | |

| · moM | 1519 | CA | GLN A | 192 | | 49.718 | | 104.412 | 1.00 20.55 |
|--------------|--------------|----------|----------------|-------|---|------------------|------------------|-----------|--------------------------|
| atom atom | 1520 | | GLN A | | | 50.474 | | 103.864 | 1.00 23.63 |
| ATOM | 1521 | CG | GLN A | | | 51.528 | 15.181 | 104.797 | 1.00 24.07 |
| | 1522 | CD | GLN A | | | 52.110 | | 104.293 | 1.00 26.90 |
| MOTA | 1523 | | GLN A | | | 52.986 | 13.860 | 103.421 | 1.00 20.21 |
| MOTA | 1524 | | GLN A | | | 51.605 | 12.765 | 104.828 | 1.00 23.52 |
| MOTA | 1525 | | GLN A | | | 48.478 | 17.174 | 103.570 | 1.00 21.41 |
| MOTA | 1525 | 0 - | GLII A | | | 47.478 | 16.466 | 103.726 | 1.00 20.15 |
| MOTA | | | SER A | | | 48.528 | 18.167 | 102.692 | 1.00 24.36 |
| MOTA | 1527 1528 | N CA | SER A | | | 47.397 | 18.448 | 101.821 | 1.00 23.98 |
| MOTA | 1529 | CB | SER A | | | 47.760 | 19.537 | 100.820 | 1.00 24.60 |
| ATOM | 1530 | OG | SER A | | • | 46.729 | 19.660 | 99.861 | 1.00 25.83 |
| MOTA | 1531 | C | SER A | | | 46.985 | 17.200 | 101.045 | 1.00 23.74 |
| MOTA | 1532 | 0 | SER A | | | 47.829 | 16.492 | 100.506 | 1.00 19.80 |
| MOTA | 1533 | N | PRO A | | | 45.674 | | 100.953 | 1.00 24.85 |
| MOTA | 1534 | CD | PRO A | | | 44.561 | 17.719 | 101.507 | 1.00 25.08 |
| MOTA MOTA | 1535 | CA | PRO A | | | 45.151 | 15.772 | 100.235 | 1.00 29.25 |
| ATOM | 1536 | CB | PRO A | | | 43.641 | 15.901 | 100.444 | 1.00 30.51 |
| ATOM | 1537 | CG | PRC A | | | 43.554 | 16.643 | 101.758 | 1.00 30.21 |
| ATOM | 1538 | c | PRO A | | | 45.527 | 15.825 | 98.756 | 1.00 30.75 |
| ATOM | 1539 | ō | PRO A | | | 45.420 | 14.830 | 98.041 | 1.00 30.04 |
| ATOM | 1540 | N | GLU A | | | 45.967 | 16.991 | 98.298 | 1.00 26.28 |
| ATOM | 1541 | CA | GLU A | 195 | | 46.343 | 17.127 | 96.898 | 1.00 31.11 |
| ATOM | 1542 | CB | GLU A | | | 46.738 | 18.570 | | 1.00 29.52 |
| MOTA | 1543 | CG | GLU A | | | 45.680 | 19.600 | 96.933 | 1.00 38.32 |
| ATOM | 1544 | CD | GLU A | | | 45.976 | 20.972 | | 1.00 44.15 |
| MOTA | 1545 | OE1 | | | | 47.139 | 21.425 | | 1.00 44.23 1.00 45.06 |
| ATOM | 1546 | OE2 | | | | 45.037 | 21.605 | | 1.00 45.06 1.00 30.81 |
| ATOM | 1547 | С | GLU A | | | 47.499 | 16.193 | | 1.00 30.81 |
| ATOM | 1548 | 0 | GLU A | | | 47.582 | 15.705 | | 1.00 37.17 |
| ATOM | 1549 | N | TYR A | | | 48.377 | 15.922 | | 1.00 23.43 |
| MOTA | 1550 | CA | TYR A | | | 49.517 | 15.053 | | 1.00 26.67 |
| MOTA | 1551 | CB | TYR A | | | 50.810 | 15.881 | | 1.00 26.78 |
| MOTA | 1552 | ÇG | TYR A | | | 51.255 | 16.424 15.625 | | 1.00 26.08 |
| MOTA | 1553 | CD1 | | | | 51.957 | 16.110 | | 1.00 26.77 |
| MOTA | 1554 | CE1 | | | | 52.338 50.944 | 17.731 | | 1.00 27.55 |
| ATOM | 1555 | CD2 | | | | 51.320 | 18.226 | | 1.00 25.95 |
| MOTA | 1556 | CE2 | | | | 52.012 | 17.409 | | 1.00 24.78 |
| ATOM | 1557 | CZ | TYR A | | | 52.356 | 17.879 | | 1.00 25.50 |
| ATOM | 1558 | OH | TYR A | 106 | | 49.670 | 13.906 | | 1.00 27.05 |
| ATOM | 1559 | C | TYR A | | | 50.585 | 13.088 | | 1.00 24.02 |
| MOTA | 1560 | 0 | TYR A ALA A | | | 48.785 | 13.822 | | 1.00 22.10 |
| ATOM | 1561 | N | ALA A | | | 48.928 | 12.760 | 100.199 | 1.00 24.90 |
| MOTA | 1562 | CA CB | ALA A | 197 | | 49.627 | 13.307 | 7 101.437 | 1.00 27.83 |
| MOTA | 1563 1534 | C | ALA | | | 47.644 | 12.069 | | 1.00 26.20 |
| ATOM | 1: 65 | ō | ALA A | 197 | | 46.553 | 12.617 | 7 100.484 | 1.00 22.82 |
| ATOM | 1556 | N | PHE A | | | 47.795 | 10.849 | 101.102 | 1.00 31.74 |
| ATCM | 1567 | CA | PHE A | | | 46.663 | 10.072 | 2 101.580 | 1.00 28.74 |
| ATOM ATOM | 1568 | CB | PHE A | | | 47.130 | 8.693 | 102.036 | 1.00 30.66 |
| ATOM | 1569 | CG | PHE A | | | 46.009 | 7.76 | | 1.00 29.61 |
| ATOM | 1570 | | PHE A | | | 45.496 | | 101.463 | 1.00 28.76 |
| ATOM | 1571 | CD2 | | 198 | | 45.426 | 7.82 | 2 103.657 | 1.00 28.43 |
| ATOM | 1572 | CEI | | | | 44.415 | 6.05 | 7 101.773 | 1.00 35.72 |
| ATOM | 1573 | CE2 | | | | 44.340 | | 4 103.970 | 1.00 34.62 |
| ATOM | 1574 | cz | | 198 | | 43.837 | 6.12 | | |
| MOTA | 1575 | c | | 198 | | 46.121 | 10.81 | | |
| ATOM | 1576 | õ | PHE A | 198 | | 46.892 | 11.34 | | |
| ATOM | 1577 | N | PRO A | 199 | | 44.792 | 10.90 | | |
| ATOM | 1578 | CD | | 199 | | 44.100 | 11.49 | | |
| ATOM | 1579 | CA | FRO 2 | A 199 | | 43.313 | 10.36 | 4 102.008 | |
| ATOM | 1580 | | PRO A | A 199 | | 42.550 | | 2 102.858 | |
| ATOM | 1581 | ĊG | PRO 2 | A 199 | | 42.665 | | | |
| ATOM | 1582 | C. | PRO 2 | A 199 | | 43.773 | | | |
| ATOM | 1583 | | PRO A | A 199 | | 44.052 | 12.63 | 1 101.280 | |
| ATOM | 1584 | N | PHE | A 200 | | 43.441 | 11.15 | 6 99.734 | 1.00 33.04 |
| | | | | | | | | | |

Figure 18-25

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 1588 1588 1588 1599 1599 1599 1599 1600 1600 1600 1611 1611 1611 1611 16 | CA PHE A 200 CB PHE A 200 CCB PHE A 200 CCCC PHE A 200 CCC CCC PHE A 200 CCC CCC CCC CCC CCC CCC CCC CCC CCC C | 43.418 43.927 45.226 46.439 46.444 47.651 47.653 42.042 41.935 41.002 39.614 39.614 39.695 39.087 | 14.460 13.729 13.318 12.854 12.663 12.290 15.101 14.666 16.152 16.862 18.986 18.717 20.017 19.416 18.075 20.017 19.416 18.075 21.103 20.377 20.329 19.267 17.329 21.103 20.786 22.337 24.695 25.954 | 102.778 102.260 100.901 99.803 99.618 98.955 98.597 97.931 103.231 104.040 103.128 103.993 103.659 104.479 105.965 104.905 102.586 101.105 102.586 101.105 100.131 99.868 100.792 98.716 | 1.00 39.87 1.00 39.94 1.00 36.58 1.00 40.98 1.00 36.30 1.00 39.98 1.00 51.87 1.00 50.32 1.00 56.69 1.00 33.85 1.00 26.22 1.00 31.68 |
|--|--|---|--|---|---|--|
| ATOM ATOM | 1639 1640 | CG GLU A 206 CD GLU A 206 | 38.307 | 23.980 23.993 | 99.868 100.792 | 1.00 51.87 1.00 50.32 |
| ATOM | 1642 | OE2 GLU A 206 | 38.581 | 23.569 | 103.427 | 1.00 33.85 |
| | | g GLU A 206 | 34.433 | 23.213 | 103.718 | 3 2.00 26.22 |
| ATOM | 1645 | N GLU A 207 | 36.071 35.297 | 21.679 20.726 | 104.599 | 1.00 31.65 |
| ATCM | 1646 1647 | CB GLU A 207 | 36.000 | 19.369 | 104.566 | 1.00 34.15 |
| ATOM ATOM | 1648 | CG GLU A 207 | 36.044 | 18.74 | 1 103.179 1 103.022 | 2 1.00 33.85 |
| ATOM | 1649 | CD GLU A 207 | 37.182 37.487 | | | |
| ATOM | 1650 | OE1 GLU A 207 | 3/.40 | . 1,02. | . = | |
| | | | | | | |

| | | | - | | 27 760 | 17 600 | 101.916 | 1.00 35.48 |
|------|------|------|---------------|---|---------|--------|-----------|--------------|
| ATOM | 1651 | OE2 | GLU A 207 | | 37.760 | 17.000 | 101.910 | |
| | 1652 | С | GLU A 207 | | 35.182 | 21.229 | 106.033 | 1.00 35.06 |
| ATOM | | | GLU A 207 | | 36.009 | 20.894 | 106.887 | 1.00 34.16 |
| ATOM | 1653 | 9 | | | | 22 024 | 106.302 | 1.00 35.99 |
| ATOM | 1654 | Ŋ | ILE A 208 | | 34.150 | | | 1.00 38.96 |
| | 1655 | CA | ILE A 208 | | 33.968 | | 107.634 | |
| MOTA | | | ILE A 208 | | 33.737 | 24.134 | 107.529 | 1.00 42.74 |
| ATOM | 1656 | CB | | | 33.717 | 24.762 | 108.914 | 1.00 48.29 |
| MOTA | 1657 | CG2. | ILE A 208 | | | | 106.700 | 1.00 40.34 |
| ATOM | 1658 | CG1 | ILE A 208 | | 34.841 | 24.795 | | 1.00 40.34 |
| | 1659 | | ILE A 208 | | 36.207 | 24.758 | | 1.00 46.23 |
| MOTA | | | ILE A 208 | | 32.821 | 21.998 | 108.452 | 1.00 38.32 |
| MOTA | 1660 | С | | | | 22.434 | 109.571 | 1.00 40.08 |
| ATOM | 1661 | 0 | ILE A 208 | • | 32.558 | | _ | 1.00 34.36 |
| ATOM | 1662 | N | GLY A 209 | | 32.142 | 20.997 | 107.901 | |
| | 1663 | CA | GLY A 209 | | 31.047 | 20.374 | 108.620 | 1.00 33.32 |
| MOTA | | | GT:17 N : 200 | | 29.699 | 20.673 | 107.993 | 1.00 37.87 |
| MOTA | 1664 | С | GLY A 209 | | 20.000 | 21.581 | 107.173 | 1.00 40.56 |
| MOTA | 1665 | 0 | GLY A 209 | | 29.579 | | | 1.00 37.38 |
| ATOM | 1666 | N | GLU A 210 | | 28.676 | | 108.380 | 1.00 37.30 |
| | | CA | GLU A 210 | | 27.337 | 20.118 | 107.831 | 1.00 42.34 |
| ATOM | 1667 | | GLU A 210 | | 27.008 | 19.012 | 106.823 | 1.00 42.73 |
| ATOM | 1668 | CB | GLU A 210 | | | 17.636 | 107.460 | 1.00 47.38 |
| ATOM | 1669 | CG | GLU A 210 | | 26.860 | | | 1.00 52.68 |
| ATOM | 1670 | CD | GLU A 210 | | 26.633 | | | |
| | 1671 | | GLU A 210 | | 26.385 | 15.379 | 106.860 | 1.00 50.59 |
| ATOM | | 051 | GLU A 210 | | 26.711 | 16.810 | 105.226 | 1.00 53.78 |
| MOTA | 1672 | | GLU A 210 | | 26.287 | 20 114 | 108.938 | 1.00 42.90 |
| ATOM | 1673 | С | GLU A 210 | | | 10 577 | 110.022 | 1.00 45.94 |
| ATOM | 1674 | 0 | GLU A 210 | | 26.516 | 19.5// | 110.022 | 1.00 43.16 |
| | 1675 | N | GLY A 211 | | 25.130 | 20.702 | 108.654 | |
| ATOM | | - | GLY A 211 | | 24.068 | 20.751 | 109.642 | 1.00 43.98 |
| MOTA | 1676 | CA | GDI A 211 | | 24.514 | 21 450 | 110.911 | 1.00 45.01 |
| ATOM | 1677 | С | GLY A 211 | | | 22.470 | 110.858 | 1.00 48.15 |
| MOTA | 1678 | 0 | GLY A 211 | | 25.186 | 22.413 | 110.050 | 1.00 41.63 |
| | 1679 | N | LYS A 212 | | 24.145 | 20.896 | 112.059 | |
| ATOM | | CA | LYS A 212 | | 24.528 | 21.495 | 113.328 | 1.00 45.07 |
| MOTA | 1680 | | 515 A 212 | | 23.913 | 20.715 | 114.490 | 1.00 46.59 |
| ATOM | 1681 | CB | LYS A 212 | | | 20 591 | 114.462 | 1.00 55.31 |
| ATOM | 1682 | CG | LYS A 212 | | 22.386 | 20.331 | 114.481 | 1.00 57.42 |
| ATOM | 1683 | CD | LYS A 212 | | 21.651 | 21.945 | 114.401 | 1.00 57.12 |
| | 1684 | CE | LYS A 212 | | 21.749 | 22.696 | 113.151 | 1.00 59.71 |
| MOTA | | | LYS A 212 | | 21.051 | 24.017 | 113.178 | 1.00 57.43 |
| ATOM | 1685 | NZ | LIS A 212 | | 26.046 | 21.513 | | 1.00 42.08 |
| ATOM | 1686 | С | LYS A 212 | | | 22.324 | 114.207 | 1.00 40.03 |
| ATOM | 1687 | 0 | LYS A 212 | | 26.598 | 22.320 | 114.207 | 1.00 39.51 |
| | 1688 | N | GLY A 213 | | 26.713 | 20.61 | 112.751 | |
| MOTA | | | GLY A 213 | | 28.163 | 20.538 | 3 112.817 | 1.00 40.11 |
| MOTA | 1689 | CA | GET A 213 | | 28.888 | 21.519 | 111.916 | 1.00 38.25 |
| ATOM | 1690 | С | GLY A 213 | | | 21 575 | 111.913 | 1.00 34.70 |
| ATOM | 1691 | 0 | GLY A 213 | | 30.122 | 21.37. | 5 111:143 | 1.00 37.31 |
| ATOM | 1692 | N | LYS A 214 | | 28.131 | 22.29 | 111.143 | 1.00 39.58 |
| | 1693 | CA | LYS A 214 | | 28.736 | 23.27 | 4 110.250 | |
| MOTA | | | LYS A 214 | | 27.656 | 24.01 | 7 109.463 | 1.00 44.69 |
| MOTA | 1694 | CB | LIS A 214 | | 28.189 | 25 03 | 0 108.461 | 1.00 44.53 |
| ATOM | 1695 | CG | LYS A 214 | | 20.103 | 25.70 | 4 107.720 | 1.00 47.71 |
| ATOM | 1696 | CD | LY: A 214 | | 27.047 | 25.70 | 2 107.750 | |
| | 1697 | CE | LY. A 214 | | 27.553 | 26.75 | 9 106.754 | 1.00 32.34 |
| MOTA | | NZ | LYL A 214 | | 28.453 | 26.18 | 3 105.717 | 1.00 57.45 |
| MOTA | 1698 | | 7 10 N 244 | | 29.547 | | 9 111.085 | 1.00 40.16 |
| MOTA | 1699 | C | LYS A 214 | | 29.002 | | 3 111.933 | 1.00 37.92 |
| ATOM | 1700 | 0 | LYS A 214 | | | | 5 110.846 | |
| ATOM | 1701 | | GLY A 215 | | 30.851 | _ | J 110.040 | |
| | 1702 | | GLY A 215 | | 31.716 | 25.18 | 3 111.593 | 1.00 35.03 |
| MOTA | | | CT 17 3 215 | | 32.431 | 24.44 | 8 112.709 | 1.00 34.57 |
| MOTA | 1703 | | GLY A 215 | | | | 9 113.454 | 1.00 33.76 |
| MOTA | 1704 | 0 | GLY A 215 | | 33.216 | | 3 112.837 | |
| MOTA | 1705 | | TYR A 216 | | 32.168 | | 2 112.03/ | |
| | | | | | 32.816 | 22.37 | 8 113.885 | |
| atom | 1706 | | | | 31.763 | 21.68 | 3 114.753 | 1.00 36.19 |
| ATOM | 1707 | | | | 30.928 | | 1 115.547 | 1.00 36.68 |
| ATOM | 1708 | CG | TYR A 216 | | 30.340 | | 2 114.925 | |
| ATOM | 1709 | | 1 TYR A 216 | | 29.961 | | 4 11F CAT | |
| | 1710 | | | | 29.249 | 24.43 | | 1.00 40.03 |
| ATOM | | | | | 31.163 | 22.86 | 9 116.910 | |
| MOTA | 1711 | | 2 11K M 210 | | 30.459 | 23.83 | 4 117.634 | 1.00 40.69 |
| ATOM | 1712 | | 2 TYR A 216 | | ,00 606 | | 2 116.994 | 1.00 40.17 |
| ATOM | 1713 | | TYR A 216 | | 29.505 | | 6 117 700 | |
| | 1714 | | TYR A 216 | | 28.816 | | 6 117.708 | 1.00 34.05 |
| MOTA | | | TYR A 216 | | 33.877 | | 4 113.40 | 1.00 34.03 |
| ATOM | 1715 | | mun 3 21c | | 34.263 | | 2 114.12 | 7 1.00 31.87 |
| MOTA | 1716 | 6 O | TYR A 216 | | 54 | | | |

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 1717 1718 1719 1720 1721 1722 1723 1724 1725 | N ASN A 217 CA ASN A 217 CB ASN A 217 CG ASN A 217 OD1 ASN A 217 ND2 ASN A 217 C ASN A 217 O ASN A 217 N LEU A 218 CA LEU A 218 CB LEU A 218 | 34.343 35.398 34.833 35.897 36.558 36.094 36.378 35.983 37.655 38.670 39.160 | 21.580 112.170 20.748 111.606 19.727 110.615 18.764 110.105 19.022 109.097 17.659 110.831 21.686 110.915 22.502 110.080 21.577 111.271 22.451 110.698 23.444 111.753 | 1.00 29.90 1.00 30.02 1.00 26.46 1.00 30.13 1.00 29.80 1.00 19.92 1.00 30.23 1.00 27.88 1.00 29.45 1.00 28.76 1.00 29.02 |
|--|--|--|--|--|--|
| MOTA MOTA | 1727 1728 | CG LEU A 218 | 39.513 | . 24.867 111.307 | 1.00 34.69 1.00 32.93 |
| ATOM | 1729 | CD1 LEU A 218 | 40.432 | 25.480 112.367 24.873 109.954 | 1.00 32.55 |
| MOTA | 1730 1731 | CD2 LEU A 218 C LEU A 218 | 39.870 | 21.657 110.207 | 1.00 26.65 |
| ATOM ATOM | 1732 | O LEU A 218 | 40.527 | 20.981 110.999 | 1.00 25.25 1.00 25.21 |
| MOTA | 1733 | N ASN A 219 | 40.151 41.287 | 21.752 108.909 21.069 108.294 | 1.00 23.21 |
| ATOM | 1734 1735 | CA ASN A 219 CB ASN A 219 | 40.875 | 20.314 107.018 | 1.00 23.69 |
| ATOM ATOM | 1736 | CG ASN A 219 | 39.972 | 19.144 107.298 | 1.00 27.88 1.00 29.28 |
| ATOM | 1737 | OD1 ASN A 219 | 40.153 39.018 | | 1.00 24.48 |
| MOTA | 1738 1739 | ND2 ASN A 219 C ASN A 219 | 42.355 | 22.074 107.906 | 1.00 23.46 |
| ATOM ATOM | 1740 | O ASN A 219 | 42.059 | | 1.00 28.17 1.00 23.90 |
| ATOM | 1741 | N ILE A 220 | 43.595 44.702 | | 1.00 23.22 |
| ATOM | 1742 1743 | CA ILE A 220 CB ILE A 220 | 45.468 | 23.131 109.212 | 1.00 28.73 |
| ATOM ATOM | 1744 | CG2 ILE A 220 | 46.601 | 24.078 108.831 | 1.00 26.01 1.00 26.36 |
| ATOM | 1745 | CG1 ILE A 220 | 44.502 43.771 | | 1.00 26.36 1.00 25.74 |
| MOTA | 1746 1747 | CD1 ILE A 220 C ILE A 220 | 45.669 | 21.929 107.018 | 1.00 25.29 |
| ATOM ATOM | 1748 | O ILE A 220 | 46.631 | 21.315 107.477 | 1.00 20.44 1.00 26.34 |
| ATOM | 1749 | N PRO A 221 | 45.396 44.234 | | 1.00 28.34 |
| ATOM | 1750 1751 | CD PRO A 221 CA PRO A 221 | 46.271 | 21.234 104.747 | 1.00 26.92 |
| ATOM ATOM | 1752 | CB PRO A 221 | 45.454 | | 1.00 27.81 |
| MOTA | 1753 | CG PRO A 221 | 44.774 47.595 | | 1.00 27.45 |
| ATOM | 1754 1755 | C PRO A 221 O PRO A 221 | 47.603 | 3 23.199 104.457 | 1.00 31.21 |
| MOTA MOTA | 1756 | N LEU A 222 | 48.704 | | 1.00 26.01 1.00 26.41 |
| MOTA | 1757 | CA LEU A 222 CB LEU A 222 | 50.038 50.726 | | 1.00 26.12 |
| atom Atom | 1758 1759 | CB LEU A 222 CG LEU A 222 | 49.960 | 22.322 107.150 | 1.00 27.67 |
| ATOM | 1760 | CD1 LEU A 222 | 50.531 | | |
| MOTA | 1761 | CD2 LEU A 222 | 50.024 50.91 | | 1.00 28.97 |
| MOTA MOTA | 1762 1763 | C LEU A 222 O LEU A 222 | 50.784 | 4 20.128 103.117 | 1.00 27.95 |
| ATOM | 1764 | N PRO A 223 | 51.82 | 1 22.116 102.964 9 23.518 103.358 | 1.00 31.52 |
| ATOM | 1765 | CD PRO A 223 CA PRO A 223 | 52.059 52.72 | 7 21.753 101.865 | 1.00 29.93 |
| ATOM ATOM | 1766 1767 | CB PRO A 223 | 53.26 | 5 23.109 101.428 | 1.00 29.16 |
| ATOM | 1768 | CG PRO A 223 | 53.45 | | |
| MOTA | 1769 | O PRO A 223 O PRO A 223 | 53.863 54.17 | 9 20.531 103.376 | 1.00 26.55 |
| ATOM ATOM | 1770 1771 | O PRO A 223 N LYS A 224 | 54.47 | 9 20.257 101.153 | 1.00 34.00 |
| ATOM | 1772 | CA LYS A 224 | 55.59 | | |
| ATOM | 1773 | CB LYS A 224 CG LYS A 224 | 55.93 54.76 | | 1.00 39.37 |
| MOTA | 1774 1775 | | 55.15 | 0 17.998 97.658 | 1.00 45.23 |
| ATOM ATOM | 1776 | CE LYS A 224 | 53.98 | | |
| ATCM | 1777 | | 54.33 56.31 | 7 20.054 101.798 | 3 1.00 29.43 |
| ATOM | 1778 1779 | | 56.93 | 3 21.270 101.640 | 1.00 24.10 |
| atom atom | 1780 | N GLY A 225 | 57.73 | 5 19.305 102.40 7 19.896 102.94 | 1.00 25.00 2 1.00 26.20 |
| ATCM | 1781 | | 58.94 58.72 | | |
| MOTA | 1782 | C GLY A 225 | 50.72 | | |

| | | | _ | | | | |
|--------------|--------------|------------------------------|---|------------------|---------|--------------------|--------------------------|
| | 4503 | O GLY A 225 | | 59.610 | 21.562 | | 1.00 29.09 |
| ATOM | | | | 57.560 | 20.679 | 104.777 | 1.00 24.26 |
| MOTA | | | | 57.212 | | 105.951 | 1.00 25.35 |
| ATOM | | | | 55.930 | 20.925 | 106.579 | 1.00 23.23 |
| ATOM | | CB LEU A 226 | | 55.172 | 21.757 | 107.611 | 1.00 28.28 |
| ATOM | | CG LEU A 226 | | 54.596 | | 106.911 | 1.00 28.07 |
| MOTA | _ | CD1 LEU A 226 | | 54.036 | | 108.226 | 1.00 27.49 |
| MOTE | | CD2 LEU A 226 | | 58.333 | | 106.998 | 1.00 24.79 |
| MOTA | 1790 | C LEU A 226 | | | | 107.299 | 1.00 26.15 |
| ATOM | | O LEU A 226 | | 58.902 58.664 | | 107.548 | 1.00 23.94 |
| ATOM | 1792 | N ASN A 227 | | 59.702 | | 108.578 | 1.00 24.89 |
| MOTA | | CA ASN A 227 | | 60.751 | | 108.269 | 1.00 27.43 |
| ATOM | | CB ASN A 227 | | 60.731 | | 108.334 | 1.00 31.62 |
| ATOM | 1795 | CG ASN A 227 | | 59.598 | | 109.336 | 1.00 31.17 |
| ATOM | 1796 | OD1 ASN A 227 | | 60.395 | 25.998 | 107.267 | 1.00 28.06 |
| ATOM | _ | ND2 ASN A 227 | | 59.076 | 22.957 | 109.960 | 1.00 23.16 |
| ATOM | 1798 | C ASN A 227 O ASN A 227 | | 57.873 | | 110.065 | 1.00 18.45 |
| MOTA | 1799 | | | 59.880 | 22.862 | 111.018 | 1.00 21.29 |
| ATOM | 1800 | | | 59.357 | 23.032 | 112.375 | 1.00 25.80 |
| MOTA | 1801 | | | 60.464 | 22.893 | 113.426 | 1.00 24.02 |
| ATOM | 1802 | CB ASP A 228 CG ASP A 228 | | 61.110 | 21.520 | 113.422 | 1.00 26.48 |
| MOTA | 1803 | OD1 ASP A 228 | | 60.410 | 20.530 | 113.135 | 1.00 29.55 |
| ATOM | 1804 | OD2 ASP A 228 | | 62.311 | 21.425 | 113.744 | 1.00 29.88 |
| MOTA | 1805 | C ASP A 228 | | 58.628 | 24.341 | 112.620 | 1.00 27.83 |
| ATOM | 1806 1807 | O ASP A 228 | | 57.589 | 24.360 | 113.284 | 1.00 25.68 |
| ATOM | 1808 | N ASN A 229 | | 59.167 | 25.437 | 112.098 | 1.00 25.78 |
| ATOM | 1809 | CA ASN A 229 | | 58.537 | 26.739 | 112.297 | 1.00 27.75 |
| MOTA | 1810 | CB ASN A 229 | | 59.453 | 27.850 | 111.770 | 1.00 32.77 |
| MOTA MOTA | 1811 | CG ASN A 229 | | 60.707 | 28.020 | 112.621 | 1.00 30.35 1.00 33.12 |
| MOTA | 1812 | OD1 ASN A 229 | | 60.635 | 28.433 | 113.782 | 1.00 33.12 1.00 28.11 |
| ATOM | 1813 | ND2 ASN A 229 | | 61.856 | 27.691 | 112.053 | 1.00 28.11 |
| ATOM | 1814 | C ASN A 229 | | 57.168 | 26.817 | 111.645 112.202 | 1.00 26.75 |
| ATOM | 1815 | O ASN A 229 | | 56.230 | 27.387 | 112.202 | 1.00 30.80 |
| ATOM | 1816 | N GLU A 230 | | 57.041 | 26:228 | 109.773 | 1.00 30.77 |
| ATOM | 1817 | CA "GLU A 230 | | 55.761 | 20.244 | 108.341 | 1.00 29.11 |
| ATOM | 1818 | CB GLU A 230 | | 55.929 | 25.710 | 107.507 | 1.00 35.94 |
| ATOM | 1819 | CG GLU A 230 | | 56.897 57.119 | 25.321 | 106.125 | 1.00 37.77 |
| ATOM | 1820 | CD GLU A 230 | | 57.465 | 24 748 | 106.039 | 1.00 38.98 |
| ATOM | 1821 | OE1 GLU A 230 | | 56.957 | | 105.129 | 1.00 31.32 |
| MOTA | 1822 | OE2 GLU A 230 C GLU A 230 | | 54.723 | 25.407 | 110.527 | 1.00 30.13 |
| MOTA | 1823 | 010 | | 53.563 | 25.799 | 110.631 | 1.00 28.35 |
| MOTA | 1824 | | | 55.141 | 24.262 | 111.060 | 1.00 32.49 |
| ATOM | 1825 | | | 54.223 | 23.386 | 111.790 | 1.00 28.54 |
| ATOM | 1826 | CA PHE A 231 CB PHE A 231 | | 54.913 | 22.075 | 112.191 | 1.00 31.22 |
| ATOM | 1827 | CG PHE A 231 | | 53.974 | 21.050 | 112.781 | 1.00 28.41 |
| ATOM | 1828 | CD1 PHE A 231 | | 53.026 | 20.417 | 111.982 | 1.00 29.66 |
| ATOM | 1829 1830 | CD2 PHE A 231 | | 54.036 | 20.723 | | |
| ATOM | 1931 | CE1 PHE A 231 | | 52.153 | 19.469 | 112.518 | |
| MOTA | 1832 | CE2 PHE A 231 | | 53.166 | | 114.681 | 1.00 31.40 1.00 30.51 |
| ATOM | 1833 | CZ PHE A 231 | | 52.223 | | 113.870 | |
| ATOM ATOM | 1834 | C PHE A 231 | | 53.693 | | 113.045 | |
| ATOM | 1835 | O PHE A 231 | | 52.483 | | 2 113.277 | |
| ATOM | 1836 | N LEU A 232 | | 54.598 | | 7 113.858 | |
| ATOM | 1837 | CA LEU A 232 | | 54.193 | | 3 115.092 | |
| ATOM | 1838 | CB LEU A 232 | | 55.422 | | 7 115.933 | |
| ATOM | 1839 | CG LEU A 232 | | 56.176 | | | |
| ATOM | 1840 | CD1 LEU A 232 | | 57.440 | | 0 117.328 | |
| ATOM | 1841 | CD2 LEU A 232 | | 55.268 | | 2 114.800 | |
| ATOM | 1842 | C LEU A 232 | | 53.37 | | 6 115.544 | |
| ATOM | | O LEU A 232 | | 52.449 | | 2 113.708 | 1.00 24.99 |
| ATOM | | N PHE A 233 | | 53.69 | | 6 113.31 | 2 1.00 28.13 |
| ATOM | 1845 | | | 52.956 53.54 | | 9 112.02 | 9 1.00 30.77 |
| ATCM | 1846 | | | 53.34 | 9 30.15 | 1 111.448 | g 1.00 29.65 |
| ATOM | 1847 | CG PHE A 233 | | 52.71 | | 1 111.96 | |
| ATCM | | CD1 PHE A 233 | | 32.00 | | | |
| | | | | | | | |

| ATOM | 1849 | CD2. PHE A 233 | | 29.903 110.412 | 1.00 31.59 |
|--------------|--------------|--------------------------------|------------------|----------------------------------|------------------------------|
| ATOM | 1850 | CE1 PHE A 233 | | 32.468 111.452 | 1.00 33.90 1.00 32.47 |
| ATOM | 1851 | CE2 PHE A 233 | | 30.924 109.895 | 1.00 32.47 |
| MOTA | 1852 | CZ PHE A 233 | 51.114 | 32.208 110.415 | 1.00 32.50 |
| ATOM | 1853 | C PHE A 233 | 51.510 | 27.999 113.031 | 1.00 25.88 |
| ATOM | 1854 | O PHE A 233 | 50.553 | 28.603 113.532 26.955 112.215 | 1.00 28.12 |
| ATOM | 1855 | N ALA A 234 | 51.370 | 26.955 112.215 26.436 111.853 | 1.00 25.68 |
| MOTA | 1856 | CA ALA A 234 | 50.056 | 25.279 110.864 | 1.00 20.08 |
| ATOM | 1857 | CB ALA A 234 | 50.195 49.304 | 25.969 113.089 | 1.00 25.17 |
| ATOM | 1858 | C ALA A 234 | 49.304 | 26.228 113.234 | 1.00 25.21 |
| ATOM | 1859 | O ALA A 234 | 50.002 | 25.285 113.987 | 1.00 28.18 |
| MOTA | 1860 | N LEU A 235 CA LEU A 235 | 49.367 | 24.781 115.195 | 1.00 33.70 |
| MOTA | 1861 | 035 | 50.356 | 23.964 116.026 | 1.00 32.70 |
| MOTA | 1862 1863 | CB LEU A 235 CG LEU A 235 | 49.772 | 22.788 116.820 | 1.00 36.89 |
| ATOM | 1864 | CD1 LEU A 235 | 50.634 | 22.545 118.052 | 1.00 31.37 |
| ATOM | 1865 | CD2 LEU A 235 | 48.344 | 23.072 117.231 | 1.00 31.47 1.00 33.38 |
| MOTA MOTA | 1866 | C LEU A 235. | 48.841 | 25.925 116.062 | 1.00 28.13 |
| MOTA | 1867 | O LEU A 235 | 47.673 | 25.926 116.455 | 1.00 28.13 |
| ATOM | 1868 | N GLU A 236 | 49.710 | 26.888 116.362 28.026 117.199 | 1.00 37.30 |
| MOTA | 18,69 | CA GLU A 236 | 49.336 | 28.026 117.133 | 1.00 41.51 |
| MOTA | 1870 | CB GLU A 236 | 50.528 51.675 | 28.356 118.188 | 1.00 49.54 |
| MOTA | 1871 | CG GLU A 236 | 52.811 | 29.334 118.451 | 1.00 55.02 |
| MOTA | 1872 | CD GLU A 236 OE1 GLU A 236 | 53.781 | 28.947 119.140 | 1.00 56.19 |
| ATOM | 1873 | OE1 GLU A 236 OE2 GLU A 236 | 52.735 | 30.486 117.968 | 1.00 54.84 |
| ATOM | 1874 1875 | C GLU A 236 | 48.163 | 28.803 116.638 | 1.00 33.98 |
| MOTA | 1876 | O GLU A 236 | 47.211 | 29.098 117.362 | 1.00 37.01 |
| MOTA MOTA | 1877 | N LYS A 237 | 48.223 | 29.137 115.354 | 1.00 33.94 1.00 33.10 |
| ATOM | 1878 | CA LYS A 237 | 47.140 | 29.888 114.726 | 1.00 36.08 |
| ATOM | 1879 | CB LYS A 237 | 47.505 | 30.244 113.281 31.186 113.165 | 1.00 33.62 |
| ATOM | 1880 | CG LYS A 237 | 48.695 | 31.186 113.165 32.508 113.856 | 1.00 37.99 |
| ATOM | 1881 | CD LYS A 237 | 48.395 | 33:471 113.762 | 1.00 45.24 |
| ATOM | 1882 | CE LYS A 237 | 49.569 49.285 | 34.737 114.500 | 1.00 43.49 |
| MOTA | 1883 | NZ LYS A 237 | 45.820 | 29.128 114.751 | 1.00 31.40 |
| MOTA | 1884 | C LYS A 237 O LYS A 237 | 44.793 | 29.680 115.131 | 1.00 31.67 |
| ATOM | 1885 | 0 LYS A 237 N SER A 238 | 45.841 | 27.861 114.354 | 1.00 28.72 |
| MOTA | 1886 1887 | CA SER A 238 | 44.610 | 27.080 114.335 | 1.00 31.74 |
| ATOM ATOM | | CB SER A 238 | 44.834 | 25.720 113.660 | 1.00 28.90 1.00 25.18 |
| ATOM | 1889 | OG SER A 238 | 45.760 | 24.924 114.372 26.891 115.740 | |
| ATOM | 1890 | C SER A 238 | 44.041 | 26.891 115.740 26.875 115.916 | |
| MOTA | 1891 | O SER A 238 | 42.823 | 26.742 116.741 | |
| ATOM | 1892 | N LEU A 239 | 44.907 44.413 | 26.587 118.108 | 1.00 37.57 |
| MOTA | 1893 | CA LEU A 239 | 45.554 | | 1.00 38.58 |
| MOTA | 1894 | CB LEU A 239 CG LEU A 239 | 46.176 | 24.907 119.038 | 1.00 39.74 |
| ATOM | 1895 | | 47.276 | 24.797 120.075 | 1.00 35.82 |
| atom | 1896 | CD2 LEU A 239 | 45.109 | 23.861 119.301 | 1.00 34.93 |
| ATOM | 1897 1898 | | 43.670 | 27.852 118.521 | 1.00 39.09 |
| MOTA MOTA | 1899 | | 42.628 | | 1.00 35.50 1.00 39.27 |
| ATOM | 1900 | | 44.202 | | |
| ATOM | 1901 | CA GLU A 240 | 43.561 | | |
| ATOM | . 1902 | CB GLU A 240 | 44.366 | | |
| ATOM | 1903 | CG GLU A 240 | 45.661 | 047 | |
| MOTA | 1904 | CD GLU A 240 | 46.407 45.772 | | |
| MOTA | 1905 | | 47.624 | | 1.00 54.05 |
| ATOM | 1906 | | 42.165 | 30.312 117.849 | 1.00 39.58 |
| ATOM | 1907 | | 42.103 | 30.822 118.45 | 5 1.00 40.99 |
| ATOM | 1908 | | 42.039 | 39.764 116.64 | 5 1.00 35.70 |
| ATCM | 1909 | | 40.754 | 29.726 115.96 | 4 1.00 38.23 |
| MOTA | 1910 | | 40.904 | 29.150 114.54 | 6 1.00 3/.55 |
| ATOM | 1911 1912 | | 39.535 | 29.005 113.89 | 5 1.00 37.30 4 1.00 38.36 |
| ATOM | 1913 | | 41.832 | 2 30.048 113./2 | |
| · ATOM | | | 42.106 | 5 29.541 112.32 | 0 1.00 50.1. |
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|--------------|--------------|----------|------------------------|--------------|------------------|---------|------------------------|--------------------------|
| | | ~ | ILE A 241 | | 39.751 | 28.881 | 116.737 | 1.00 37.31 |
| ATOM | 1915 | C | ILE A 241 | | 38.591 | 29.264 | 116.884 | 1.00 37.91 |
| ATOM | 1916 | 0 | VAL A 242 | | 40.203 | 27.732 | 117.231 | 1.00 37.07 |
| MOTA | 1917 | N | VAL A 242 | | 39.336 | 26.832 | 117.981 | 1.00 38.35 |
| MOTA | 1918 | CA | VAL A 242 | | 40.025 | 25.477 | 118.250 | 1.00 37.58 |
| MOTA | 1919 | CB | VAL A 242 | | 39.120 | 24.581 | 119.078 | 1.00 31.91 |
| MOTA | 1920 | CG1 | VAL A 242 | | 40.364 | | 116.928 | 1.00 39.21 |
| ATOM | 1921 | | VAL A 242 | | 38.930 | | 119.305 | 1.00 40.40 |
| MOTA | 1922 | C | VAL A 242 | | 37.759 | 27.422 | 119.675 | 1.00 38.19 |
| MOTA | 1923 | 0 | VAL A 242 | | | 29 008 | 120.014 | 1.00 45.47 |
| ATOM | 1924 | N | LYS A 243 | | 39.905 39.661 | 20.000 | 121.301 | 1.00 48.74 |
| MOTA | 1925 | CA | | • | 40.945 | 20.034 | 121.801 | 1.00 51.01 |
| ATOM | 1926 | CB | LYS A 243 | | 40.943 | 28 426 | 122.614 | 1.00 56.09 |
| MOTA | 1927 | CG | LYS A 243 | | 41.250 | 28 149 | 123.991 | 1.00 57.39 |
| MOTA | 1928 | CD | LYS A 243 | | 41.054 | 29.436 | 124.783 | 1.00 59.53 |
| MOTA | 1929 | CE | LYS A 243 LYS A 243 | | 40.448 | 29.193 | 126.127 | 1.00 57.91 |
| MOTA | 1930 | NZ | LYS A 243 | | 38.559 | | 121.260 | 1.00 51.67 |
| MOTA | 1931 | C | LYS A 243 | | 37.815 | 29.871 | 122.226 | 1.00 52.84 |
| MOTA | 1932 | 0 | GLU A 244 | | 38.451 | 30.410 | 120.140 | 1.00 53.77 |
| MOTA | 1933 | N | GLU A 244 | | 37.460 | 31.471 | 120.004 | 1.00 54.74 |
| ATOM | 1934 | CA | GLU A 244 | | 37.954 | 32.497 | 118.986 | 1.00 55.15 |
| MOTA | 1935 | CB CG | GLU A 244 | | 37.068 | 33.717 | 118.865 | 1.00 60.63 |
| ATOM | 1936 | CD | GLU A 244 | | 37.602 | 34.714 | 117.868 | 1.00 65.87 |
| ATOM | 1937 1938 | CEI | | | 38.746 | 35.181 | 118.053 | 1.00 70.36 |
| ATOM | 1939 | OE2 | | | 36.879 | 35.031 | 116.900 | 1.00 67.09 1.00 52.65 |
| ATOM | 1940 | C | GLU A 244 | | 36.051 | 31.025 | 119.626 | 1.00 52.65 |
| MOTA MOTA | 1941 | Ö | GLU A 244 | | 35.127 | 31.838 | 119.606 | 1.00 55.59 |
| ATOM | 1942 | N | VAL A 245 | | 35.869 | 29.745 | 119.332 | 1.00 50.57 |
| ATOM | 1943 | CA | VAL A 245 | | 34.546 | 29.269 | 118.947 | 1.00 45.75 |
| ATOM | 1944 | СВ | VAL A 245 | | 34.475 | 29.081 | 117.409 | 1.00 46.91 |
| MOTA | 1945 | CG1 | | | 33.085 | 28.634 | 116.986 | 1.00 52.62 1.00 48.34 |
| ATOM | 1946 | CG2 | VAL A 245 | | 34.825 | 30.389 | 116.716 | 1.00 48.34 |
| MOTA | 1947 | С | VAL A 245 | | 34.130 | 27.969 | 119.642 | 1.00 43.61 |
| MOTA | 1948 | 0 | VAL A 245 | | 33.021 | 27.480 | 119.445 | 1.00 40.87 |
| ATOM | 1949 | N | PHE A 246 | | 35.001 | 27.417 | 120.477 | 1.00 37.47 |
| ATOM | 1950 | CÃ | PHE A 246 | | 34.662 | 26.100 | 120.257 | 1.00 37.00 |
| MOTA | 1951 | СB | PHE A 246 | | 35.106 | 24.551 | 120.604 | 1.00 33.22 |
| MOTA | 1952 | CG | PHE A-246 | | 34.450 | 23.003 | 120.302 | 1.00 33.93 |
| ATOM | 1953 | | 1 PHE A 246 | | 33.111 35.168 | 22 674 | 121.234 | |
| MOTA | 1954 | CD: | | | 32.493 | 22.260 | 120.621 | 1.00 37.75 |
| ATOM | 1955 | CE: | | | 34.561 | 21.459 | 121.561 | 1.00 35.92 |
| MOTA | 1956 | CE | 2 PHE A 246 | | 33.217 | 21.252 | 121.251 | 1.00 36.30 |
| MOTA | 1957 | CI | PHE A 246 PHE A 246 | | 35.322 | 26.069 | 122.509 | 1.00 38.93 |
| ATOM | 1958 | C | PHE A 246 | | 36.546 | 26.158 | 3 122.630 | 1.00 40.66 |
| ATOM | 1959 | 0 | GLU A 247 | | 34.500 | 25.870 | 123.537 | 1.00 38.59 |
| MOTA | 1960 | N CA | | | 34.970 | 5.73 | 3 124.918 | 1.00 44.60 |
| MOTA | 1961 | CB | | | 34.146 | 5.61 | 5 125.865 | 1.00 47.07 |
| ATOM | 1962 | CG | | | 33.161 | 27.56 | 9 125.185 | 1.00 56.16 |
| MOTA | 1963 1964 | 22 | | | 31.944 | 26.86 | 5 124.577 | 1.00 62.03 |
| ATOM | 1965 | ೧೯ | 1 GLU A 247 | | 32.096 | | 8 123.607 | 1.00 61.85 |
| ATOM | 1966 | ΩE | | | 30.822 | 27.09 | 4 125.083 | 1.00 64.59 |
| ATOM ATOM | 1967 | Ē | GLU A 247 | | 34.774 | 24.26 | 9 125.285 | 1.00 39.40 |
| ATOM | 1968 | | GLU A 247 | | 33.727 | | 9 125.794 | 1.00 39.91 1.00 38.64 |
| MOTA | 1969 | | PRO A 248 | | 35.792 | | 2 125.041 | |
| ATOM | 1970 | | PRO A 248 | | 37.101 | | | |
| ATOM | 1971 | | PRO A 248 | | 35.769 | | 6 125.316 1 124.648 | |
| ATOM | 1972 | CE | PRO A 248 | | 37.047 | 21.53 | | |
| ATOM | 1973 | | PRO A 248 | | 37.970 | 22.68 | | |
| ATOM | 1974 | | PRO A 248 | | 35.736 | | 6 127.597 | |
| ATOM | 1975 | 2 | PRO A 248 | } | 36.445 | | 6 127.096 | |
| ATOM | 1976 | | GLU A 249 |) | 34.914 | | 5 128.459 | |
| ATOM | 1977 | | GLU A 249 |) | 34.841 | | | |
| MOTA | 1978 | | | , | 33.521 | | | 1.00 35.98 |
| ATOM | 1979 | | GLU A 249 |) | 32.284 31.026 | | 8 128.668 | |
| ATCM | 1980 |) c: | GLU A 249 | , | 21.020 | . 13.30 | | • |
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|--------------|--------------|--------------------------------|--------------------|----------------------------------|--------------------------|
| ATOM | 1981 | OE1 GLU A 249 | | 18.509 127.804 19.609 129.620 | 1.00 40.27 1.00 38.57 |
| ATOM | 1982 | OE2 GLU A 249 | | | 1.00 32.30 |
| MOTA | 1983 | C GLU A 249 | | 19.119 128.623 | 1.00 28.51 |
| ATOM | 1984 | O GLU A 249 | 36.472 | 18.884 129.728 | 1.00 23.31 |
| MOTA | 1985 | N VAL A 250 | 36.434 | 18.547 127.502 | 1.00 29.31 |
| ATOM- | 1986 | CA VAL A 250 | 37.516 | 17.563 127.494 | 1.00 29.85 |
| ATOM | 1987 | CB VAL A 250 | 36.988 | 16.174 127.926 | 1.00 24.36 |
| ATOM | 1988 | CG1 VAL A 250 | 35.908 | 15.711 126.958 15.166 127.978 | 1.00 25.60 |
| ATOM | 1989 | CG2 VAL A 250 | 38.121 | | 1.00 29.30 |
| ATOM | 1990 | C VAL A 250 | 38.066 | 17.453 126.076 17.741 125.114 | 1.00 24.46 |
| ATOM | 1991 | O VAL A 250 | 37.358 | 17.046 125.930 | 1.00 27.96 |
| ATOM | 1992 | N TYR A 251 | 39.323 | 16.913 124.585 | 1.00 30.06 |
| MOTA | 1993 | CA TYR A 251 | - 39.865 40.585 | 18.206 124.165 | 1.00 25.89 |
| MOTA | 1994 | CB TYR A 251 | 41.998 | 18.370 124.692 | 1.00 29.90 |
| MOTA | 1995 | CG TYR A 251 | 43.087 | 17.794 124.029 | 1.00 26.02 |
| MOTA | 1996 | CD1 TYR A 251 | 44.390 | 17.953 124.507 | 1.00 29.20 |
| ATOM | 1997 | CE1 TYR A 251 CD2 TYR A 251 | 42.249 | 19.107 125.849 | 1.00 31.96 |
| ATOM | 1998 | | 43.551 | 19.271 126.338 | 1.00 31.54 |
| MOTA | 1999 | | 44.614 | 18.694 125.664 | 1.00 31.46 |
| ATOM | 2000 | CZ TYR A 251 OH TYR A 251 | 45.894 | 18.854 126.152 | 1.00 29.69 |
| ATOM | 2001 2002 | C TYR A 251 | 40.801 | 15.731 124.451 | 1.00 27.56 |
| MOTA | 2002 | O TYR A 251 | 41.382 | 15.273 125.436 | 1.00 28.23 |
| MOTA | 2003 | N LEU A 252 | 40.908 | 15.222 123.227 | 1.00 23.52 |
| MOTA MOTA | 2005 | CA LEU A 252 | 41.806 | 14.117 122.919 | 1.00 26.53 |
| ATOM | 2006 | CB LEU A 252 | 41.057 | 12.930 122.293 | 1.00 25.74 |
| MOTA | 2007 | CG LEU A 252 | 40.266 | 12.001 123.221 | 1.00 28.49 1.00 27.67 |
| ATOM | 2008 | CD1 LEU A 252 | 39.122 | 12.753 123.868 | 1.00 27.87 |
| ATOM | 2009 | CD2 LEU A 252 | 39.727 | 10.835 122.414 | 1.00 32.00 |
| ATOM | 2010 | C LEU A 252 | 42.842 | 14.638 121.932 15.444 121.055 | 1.00 24.42 |
| ATOM | 2011 | O LEU A 252 | 42.528 | 14.176 122.078 | 1.00 24.60 |
| MOTA | 2012 | N LEU A 253 | 44.075 45.157 | 14.599 121.204 | 1.00 25.04 |
| MOTA | 2013 | CA LEU A 253 | 46.176 | 15.400 122.017 | 1.00 22.48 |
| ATOM | 2014 | CB LEU A 253. | 47.456 | 15.880 121.323 | 1.00 21.05 |
| MOTA | 2015 | CG LEU A 253 CD1 LEU A 253 | 47.105 | 16.833 120.175 | 1.00 23.05 |
| ATOM | 2016 | CD2 LEU A 253 | 48.348 | 16.578 122.360 | 1.00 16.40 |
| ATOM | 2017 | C LEU A 253 | 45.822 | 13.374 120.580 | 1.00 23.55 |
| ATOM | 2018 2019 | O LEU A 253 | 46.329 | 12.516 121.303 | 1.00 22.11 |
| MOTA | 2020 | N GLN A 254 | 45.811 | 13.287 119.248 | 1.00 22.33 |
| MOTA MOTA | 2021 | CA GLN A 254 | 46.417 | 12.150 118.552 | 1.00 19.84 1.00 23.09 |
| ATOM | 2022 | CB GLN A 254 | 45.542 | 11.731 117.348 | 1.00 25.09 |
| ATOM | 2023 | CG GLN A 254 | 46.075 | 12.038 115.963 | 1.00 33.45 |
| ATOM | 2024 | CD GLN A 254 | 47.073 | 11.017 115.453 9.937 114.961 | 1.00 33.69 |
| ATOM | 2025 | OE1 GLN A 254 | 46.712 | | 1.00 31.02 |
| TOM | 2026 | NE2 GLN A 254 | 48.338 | 11.349 115.574 12.576 118.153 | 1.00 22.46 |
| .TOM | 2027 | C GLN A 254 | 47.831 | 13.599 117.478 | 1.00 17.56. |
| r.rom | 2028 | O GLN A 254 | 48.034 48.804 | 11.781 118.590 | 1.00 17.64 |
| ATOM | 2029 | N LEU A 255 | 50.213 | 12.079 118.383 | 1.00 17.04 |
| MOTA | 2030 | CA LEU A 255 | 50.894 | 12.136 119.750 | 1.00 14.75 |
| MOTA | 2031 | CB LEU A 255 CG LEU A 255 | 50.277 | 13.196 120.670 | 1.00 25.02 |
| ATOM | 2032 | CG LEU A 255 CD1 LEU A 255 | 50.732 | 12.996 122.107 | 1.00 21.99 |
| ATOM | 2033 | CD2 LEU A 255 | 50.636 | 14.578 120.149 | 1.00 18.30 |
| MOTA | 2034 | C LEU A 255 | 51.023 | .11.169 117.476 | 1.00 21.34 |
| MOTA | 2035 2036 | 0.55 | 52.089 | 10.705 117.875 | 1.00 18.73 |
| ATOM | 2037 | | 50.543 | 10.928 116.259 | 1.00 22.75 |
| MOTA | 2037 | | 51.291 | 10.093 115.330 | 1.00 24.09 |
| MOTA MOTA | 2039 | | 52.660 | | 1.00 24.27 1.00 19.15 |
| ATOM | 2040 | O GLY A 256 | 52.805 | | |
| ATOM | 2041 | N THR A 257 | 53.680 | | |
| ATOM | 2042 | CA THR A 257 | 55.014 | | |
| MOTA | 2043 | CB THR A 257 | 56.048 | | |
| ATOM | 2044 | OG1 THR A 257 | 56.009 | | |
| ATOM | 2045 | CG2 THR A 257 | 55.728 | | |
| ATOM | 2046 | C THR A 257 | 55.403 | 10.321 140.430 | |

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|--------------|--------------|----------|----------------|----------------|-----|------------------|--------|------------------------|--------------------------------|
| ATOM | 2047 | о т | THR A | 257 | 56 | .517 | 10.941 | 112.974 | 1.00 20.39 |
| ATOM | 2048 | N A | ASP A | 258 | _ | .493 | 10.177 | 112.379 | 1.00 22.20 |
| ATOM | 2049 | CA A | ASP A | 258 | | .863 | | 110.961 110.056 | 1.00 25.06 |
| MOTA | 2050 | | ASP A | | | .849 | 9.496 | | |
| MOTA | 2051 | | ASP A | | | .415 | | 110.252 | |
| MOTA | 2052 | C P | ASP A | 258 | | .222 .756 | 11 661 | 109.254 | |
| MOTA | 2053 | | ASP A | | | 2.173 | 11 070 | 110.742 | |
| ATOM | 2054 | | ASP A | | | .513 | 9.168 | 109.869 | 1.00 33.25 |
| MOTA | 2055 | N I | ASP A PRO A | 200 250 | | 1.884 | 12.710 | 111.045 | 1.00 31.06 |
| ATOM | 2056 2057 | | PRO A | | | .019 | 12.928 | 3 112.220 | 1.00 28.59 |
| MOTA MOTA | 2058 | | PRO A | | 5 | 5.268 | 14.006 | | |
| ATOM | 2059 | | PRO A | | _ | 1.447 | 14.99 | | |
| ATOM | 2060 | CG I | PRO A | 259 | | 4.418 | 14.32 | | |
| MOTA | 2061 | C 1 | PRO A | 259 | | 5.790 | 14.26 | 1 110.044 | |
| MOTA | 2062 | 0 1 | PRO A | 259 | | 7.300 7.508 | 13.38 | 111.280 | |
| ATOM | 2063 | | LEU A | | | 8.960 | 13.54 | | 5 1.00 28.41 |
| ATOM | 2064 2065 | | LEU A | | | 9.461 | 12.57 | | 3 1.00 22.47 |
| ATOM | 2066 | | LEU A | | | 8.970 | 12.79 | | |
| MOTA MOTA | 2067 | CD1 | LEU A | 260 | | 9.352 | 11.59 | | |
| ATOM | 2068 | CD2 | LEU A | 260 | | 9.592 | 14.07 | 9 114.53 | |
| MOTA | 2069 | | LEU A | | 5 | 9.770 | 13.34 | | |
| MOTA | 2070 | | LEU A | | | 9.407 | | 1 110.04 | |
| MOTA | 2071 | | LEU A | | | 0.874 1.742 | 14.01 | | |
| ATOM | 2072 | | LEU A | | | 3.067 | 14.73 | 7 109.13 | |
| MOTA | 2073 2074 | | LEU A | | | 4.131 | 14.61 | 5 108.02 | 5 1.00 29.52 |
| ATOM ATOM | 2075 | | LEU A | | 6 | 3.642 | 15.32 | 5 106.77 | 0 1.00 22.68 |
| ATOM | 2076 | CD2 | LEU A | 261 | | 5.460 | 15.21 | 9 108.47 | 5 1.00 26.71 3 1.00 28.23 |
| ATOM | 2077 | | LEU A | | 6 | 2.063 | 12.57 | 7 108.44 8 107.28 | |
| MOTA | 2078 | | LEU A | 261 | | 1.880 | 11 78 | 7. 109.39 | |
| MOTA | 2079 | | GLU A GLU A | | | 2.938 | 10.41 | 6 109.13 | 5 1.00 31.76 |
| ATOM | 2080 | | GLU A | | | 3.685 | 9.85 | 5 110.35 | 1.00 29.72 |
| MOTA MOTA | 2081 2082 | CG | GLU A | | 6 | 4.890 | 10.68 | 3 110.80 | 3 1.00 31.33 |
| MOTA | 2083 | CD | GLU A | 262 | | 4.521 | 11.84 | 7 111.70 | 1.00 28.07 1.00 28.75 |
| ATOM | 2084 | | | | | 3.324 | 12.19 | 5 111.78 4 112.34 | |
| MOTA | 2085 | | GLU A | | | 5.433 | 9.42 | | |
| MOTA | 2086 | C | GLU A | | | 2.158 | 8.30 | | 1.00 29.72 |
| ATOM | 2087 2088 | о И | ASP A | | è | 0.582 | 9.82 | 25 108.78 | |
| MOTA MOTA | 2089 | CA | ASP A | 263 | 5 | 9.513 | 8.90 | 2 108.47 | 1.00 26.85 |
| ATOM | 2090 | CB | ASP A | 263 | | 8.305 | 9.09 | 9 109.33 | 33 1.00 25.26 35 1.00 33.14 |
| ATOM | 2091 | CG | ASP A | 263 | | 7.261 | 7.99 | 98 109.18 36 110.20 | |
| ATOM | 2092 | OD1 | ASP A | 263 | | 6.638 | 7.6. | 09 108.05 | |
| MOTA | 2093 | | ASP A | 263 | | 57.042 59.150 | 9.1 | 16 106.9 | |
| ATOM | 2094 | C | ASP A | 263 | | 5B.740 | 10.2 | 17 106.5 | 94 1.00 24.70 |
| ATOM | 2095 | 0 N | TYR A | 264 | | 59.303 | 8.1 | 11 106.13 | 30 1.00 27.51 |
| ATOM | 2096 2097 | CA | TYR A | 264 | ! | 59.031 | 8.2 | 19 104 6 | 96 1.00 33.89 |
| MOTA MOTA | 2098 | CB | TYR A | 264 | ! | 59.576 | 7.0 | 08 103.9 | 35 1.00 40.44 92 1.00 50.64 |
| ATOM | 2099 | CG | TYR A | 264 | | 51.059 | _ | 71 104.0 | |
| ATOM | 2100 | | TYR A | 264 | | 61.565 | | 87 105.1 76 105.3 | |
| MOTA | 2101 | CE1 | TYR A | 264 | | 62.933 61.960 | | 42 103.1 | 40 1.00 53.79 |
| ATOM | 2102 | | TYR A | 264 | | 63.329 | | 38 103.2 | 82 1.00 56.61 |
| MOTA | 2103 | CE2 | TYR A | 264 | | 63.809 | 6.3 | 54 104.3 | 88 1.00 56.22 |
| MOTA | 2104 2105 | CZ OH | TYR A | 264 | | 65.161 | 6.1 | 47 104.5 | 24 1.00 55.90 |
| MOTA MOTA | 2105 | | TYR A | 264 | | 57.581 | 8.3 | 94 104.2 | 94 1.00 31.33 78 1.00 27.15 |
| ATOM | 2107 | ō | TYR F | 264 | | 57.311 | | 25 103.1 | |
| ATOM | 2108 | | LEU A | 265 | | 56.641 | | 59 105.1 09 104.7 | |
| ATOM | 2109 | CA | LEU A | 265 | | 55.244 54.360 | | 89 105.5 | 27 1.00 26.55 |
| ATOM | 2110 | | LEU A | 265 | | 54.360 54.663 | | 24 105.1 | 68 1.00 29.80 |
| MOTA | 2111 | | LEU A | 4 265 4 265 | | 53.464 | | | 03 1.00 21.17 |
| MOTA | 2112 | עט | . <u>.</u> 2 | . 200 | | | | | |
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|--------------|--------------|------------------------------|--------------|-----------|------------------------|--------------------------|
| | | CD2 LEU A 265 | 54.93 | 1 5.620 | 103.682 | 1.00 33.35 |
| MOTA | 2113 | | 54.66 | | 104.921 | 1.00 20.81 |
| ATOM | 2114 | | 53.45 | | 104.979 | 1.00 21.30 |
| MOTA | 2115 | | 55.54 | | 104.959 | 1.00 23.23 |
| MOTA | 2116 | N SER A 266 | 55.08 | | 105.008 | 1.00 26.30 |
| ATOM | 2117 | CA SER A 266 | 54.85 | | 106.444 | 1.00 25.16 |
| MOTA | 2118 | CB SER A 266 | | ▼ | 107.084 | 1.00 22.92 |
| MOTA | 2119 | OG SER A 266 | 56.07 | | | 1.00 30.17 |
| ATOM | 2120 | C SER A 266 | 56.14 | | | 1.00 31.65 |
| ATOM | 2121 | O SER A 266 | 57.33 | | 103.757 | 1.00 31.56 |
| ATOM | 2122 | N LYS A 267 | 55.73 | | 103.737 | 1.00 27.65 |
| MOTA | 2123 | CA LYS A 267 | 56.69 | | | 1.00 30.54 |
| ATOM | 2124 | CB LYS A 267 | 56.14 | 0 15.425 | | 1.00 34.13 |
| ATOM | 2125 | CG LYS A 267 | 55.81 | | | 1.00 29.09 |
| MOTA | 2126 | CD LYS A 267 | 57.03 | | | 1.00 37.61 |
| ATOM | 2127 | CE LYS A 267 | 56.74 | | 99.324 | 1.00 31.91 |
| ATOM | 2128 | NZ LYS A 267 | 57.95 | | | 1.00 30.85 |
| MOTA | 2129 | C LYS A 267 | 57.09 | | - - | 1.00 27.86 |
| MOTA | 2130 | O LYS A 267 | 57.62 | | | 1.00 24.19 |
| ATOM | 2131 | N PHE A 268 | 56.68 | | | 1.00 25.34 |
| ATOM | 2132 | CA PHE A 268 | 57.00 | | | 1.00 24.54 |
| ATOM, | 2133 | CB PHE A 268 | 56.0 | | | 1.00 21.68 |
| ATOM | 2134 | CG PHE A 268 | 54.63 | 36 17.256 | 107.257 | 1.00 28.65 |
| ATOM | 2135 | CD1 PHE A 268 | 53.63 | 31 17.221 | 108.216 | 1.00 25.14 |
| MOTA | 2136 | CD2 PHE A 268 | 54.3 | | 106.011 | 1.00 25.34 |
| MOTA | 2137 | CE1 PHE A 268 | 52.3 | | 107.944 | 1.00 23.79 |
| ATOM | 2138 | CE2 PHE A 268 | 53.0 | | 105.730 | 1.00 28.13 |
| MOTA | 2139 | CZ PHE A 268 | 52.0 | | 106.702 | 1.00 25.66 |
| ATOM | 2140 | C PHE A 268 | 58.4 | | 106.908 | 1.00 28.44 |
| ATOM | 2141 | O PHE A 268 | 58.7 | | 107.230 | 1.00 25.81 |
| MOTA | 2142 | N ASN A 269 | 59.1 | | 107.709 | 1.00 30.60 |
| ATOM | 2143 | CA ASN A 269 | 60.5 | | | 1.00 31.97 |
| MOTA | 2144 | CB ASN A 269 | 61.5 | | | 1.00 35.83 |
| MOTA | 2145 | CG ASN A 269 | 61.2 | | | 1.00 33.93 |
| ATOM | 2146 | OD1 ASN A 269 | 61.4 | | | 1.00 33.95 |
| ATOM | 2147 | ND2 ASN A 269 C ASN A 269 | 60.7 | | 3 109.110 | 1.00 31.80 |
| ATOM | 2148 | 0 60 | 61.6 | | 5 109.348 | 1.00 28.13 |
| MOTA | 2149 | | 59.8 | 88 17.39 | 7 110.043 | 1.00 29.70 |
| ATOM | 2150 | CA LEU A 270 | 59.9 | 54 17.91 | 8 111.406 | 1.00 26.87 |
| MOTA | 2151 2152 | CB LEU A 270 | 58.5 | | | 1.00 26.60 |
| MOTA | 2152 | CG LEU A 270 | 57.3 | 92 18.42 | 5 111.297 | 1.00 29.62 |
| ATOM | 2154 | CD1 LEU A 270 | 56.1 | | 4 112.222 | 1.00 28.54 1.00 29.40 |
| ATOM ATOM | 2155 | CD2 LEU A 270 | 57.7 | | | 1.00 26.83 |
| ATOM | 3156 | C LEU A 270 | 60.9 | | 2 112.301 | |
| ATOM | 2157 | O LEU A 270 | 61.4 | | 8 111.990 | |
| ATOM | 2158 | N SER A 271 | 61.2 | | 6 113.420 5 114.393 | 1.00 27.08 |
| ATOM | 2159 | CA SER A 271 | 62.2 | | 0 114.846 | |
| ATOM | 2160 | CB SER A 271 | 63.1 | | 3 115.626 | |
| ATOM | 2161 | OG SER A 271 | 62.4 | | 8 115.618 | |
| ATOM | 2162 | | 61.4 | | 0 115.772 | |
| ATCM | 2163 | | 60.2 | | 9 116.470 | |
| MOTA | 2164 | | 62.3 61.0 | | 13 117.739 | 1.00 31.03 |
| MOTA | 2165 | | 62. | | | 1.00 28.80 |
| MOTA | 2166 | | 62. | | | 1.00 36.65 |
| MOTA | 2167 | | 63. | | | 1.00 29.89 |
| ATOM | 2168 | OD1 ASN A 272 | | | | 1.00 40.80 |
| ATOM | 2169 | | | | | 1.00 31.83 |
| ATOM | 2170 |) C ASN A 272 | | | | 1.00 27.50 |
| ATOM | 2171 | O ASN A 272 | | | 3 118.804 | 1.00 31.49 |
| atom | 2172 | N VAL A 273 CA VAL A 273 | | | 37 119.667 | 1.00 31.58 |
| ATOM | 2173 | | | | 09 119.725 | 1.00 35.80 |
| ATOM | 2174 | | | 804 20.9 | | 1.00 48.07 |
| ATOM | 2175 2176 | | 64. | 198 18.9 | 14 120.38 | 1.00 42.81 |
| ATOM | 2177 | | 60. | 608 19.6 | 65 119.23 | 1.00 30.13 |
| ATCM | 2178 | | | 872 20.1 | 74 120.07 | 2 1.00 31.44 |
| ATOM | | V V V | _ | | | |

| 3 mom | 2179 | N ALA A 274 | 60.405 | 19.800 117.929 | 1.00 24.15 |
|--------------|--------------|-------------------------------|------------------|----------------------------------|--------------------------|
| MOTA MOTA | 2180 | CA ALA A 274 | 59.258 | 20.558 117.455 | 1.00 26.27 |
| ATOM | 2181 | CB ALA A 274 | 59.341 | 20.780 115.965 | 1.00 21.85 |
| ATOM | 2182 | C ALA A 274 | 58.005 | 19.759 117.789 | 1.00 25.68 |
| ATOM | 2183 | O ALA A 274 | 56.961 | 20.324 118.132 | 1.00 23.76 |
| ATOM | 2184 | N PHE A 275 | 58.122 | 18.438 117.680 | 1.00 25.20 |
| MOTA | 2185 | CA PHE A 275 | 57.015 | 17.538 117.974 | 1.00 25.89 1.00 25.21 |
| MOTA | 2186 | CB PHE A 275 | 57.449 | 16.092 117.710 | 1.00 25.21 |
| ATOM | 2187 | CG PHE A 275 | 56.340 | 15.088 117.870 15.064 116.982 | 1.00 28.63 |
| ATOM | 2188 | CD1 PHE A 275 | 55.278 | 15.064 116.982 14.166 118.910 | 1.00 28.93 |
| MOTA | 2189 | CD2 PHE A 275 | . 56.365 | 14.132 117.119 | 1.00 33.75 |
| MOTA | 2190 | CE1 PHE A 275 | 54.248 | 13.231 119.059 | 1.00 30.83 |
| MOTA | 2191 | CE2 PHE A 275 | 55.343 54.282 | 13.214 118.160 | 1.00 34.19 |
| MOTA | 2192 | CZ PHE A 275 C PHE A 275 | 56.607 | 17.712 119.445 | 1.00 24.63 |
| MOTA | 2193 | O PHE A 275 | 55.428 | 17.877 119.767 | 1.00 22.40 |
| MOTA | 2194 2195 | N LEU A 276 | 57.594 | 17.673 120.331 | 1.00 25.45 |
| ATOM | 2195 | CA LEU A 276 | 57.357 | 17.837 121.766 | 1.00 27.94 |
| ATOM | 2197 | CB LEU A 276 | 58.667 | 17.692 122.534 | 1.00 26.11 |
| ATOM ATOM | 2198 | CG LEU A 276 | 58.651 | 18.132 124.001 | 1.00 31.15 |
| ATOM | 2199 | CD1 LEU A 276 | 57.609 | 17.351 124.761 | 1.00 29.37 |
| ATOM | 2200 | CD2 LEU A 276 | 60.033 | 17.937 124.612 | 1.00 27.98 1.00 30.12 |
| ATOM | 2201 | C LEU A 276 | 56.770 | 19.208 122.058 | 1.00 30.12 |
| ATOM | 2202 | O LEU A 276 | 55.822 | 19.348 122.838 | 1.00 28.09 |
| ATOM | 2203 | N LYS A 277 | 57.353 | 20.219 121.425 21.593 121.603 | 1.00 27.04 |
| MOTA | 2204 | CA LYS A 277 | 56.913 | 22.516 120.704 | 1.00 30.38 |
| MOTA | 2205 | CB LYS A 277 | 57.742 57.941 | 23.934 121.237 | 1.00 36.46 |
| MOTA | 2206 | CG LYS A 277 | 57.941 | 24.668 121.454 | 1.00 42.73 |
| MOTA | 2207 | CD LYS A 277 CE LYS A 277 | 56.870 | 26.059 122.049 | 1.00 45.70 |
| MOTA | 2208 | | 57.528 | 26.004 123.390 | 1.00 44.64 |
| ATOM | 2209 2210 | NZ LYS A 277 C LYS A 277 | 55.432 | 21.683 121.242 | 1.00 30.26 |
| MOTA | 2210 | O LYS A 277 | 54.640 | 22.284 121.972 | 1.00 27.55 |
| MOTA MOTA | 2212 | N ALA A 278 | 55.057 | 21.078 120.115 | 1.00 30.15 |
| ATOM | 2213 | CA ALA A 278 | 53.662 | 21.096 119.676 | 1.00 30.51 |
| MOTA | 2214 | CB ALA A 278 | 53.496 | 20.270 118.406 | 1.00 28.96 1.00 30.99 |
| MOTA | 2215 | C ALA A 278 | 52.789 | 20.527 120.786 | 1.00 30.39 |
| ATOM | 2216 | O ALA A 278 | 51.735 | 21.067 121.108 19.422 121.360 | 1.00 27.85 |
| ATOM | 2217 | N PHE A 279 | 53.245 | 18.759 122.448 | 1.00 29.62 |
| ATOM | , 2218 | CA PHE A 279 | 52.540 53.343 | 17.534 122.886 | 1.00 26.83 |
| MOTA | 2219 | CB PHE A 279 | 52.786 | 16.823 124.078 | 1.00 29.11 |
| ATOM | 2220 | CG PHE A 279 CD1 PHE A 279 | 51.556 | 16.176 124.015 | 1.00 28.86 |
| MOTA | 2221 | CD1 PHE A 279 | 53.505 | 16.786 125.267 | 1.00 33.03 |
| MOTA | 2222 2223 | CE1 PHE A 279 | 51.054 | 15,500 125,121 | 1.00 37.90 |
| ATOM | 2224 | CE2 PHE A 279 | 53.011 | 16.114 126.386 | 1.00 38.01 |
| MOTA MOTA | 2225 | CZ PHE A-279 | 51.783 | 15.469 126.313 | 1.00 36.33 |
| ATOM | 2226 | C PHE A 279 | | 19.730 123.621 | 1.00 30.57 |
| ATOM | 2227 | O PHE A 279 | 51.265 | 19.853 124.184 | 1.00 26.26 |
| ATOM | 2228 | N ASN A 280 | 53.432 | 20.429 123.990 | 1.00 32.03 |
| MOTA | 2229 | CA ASN A 280 | 53.339 | | 1.00 36.79 |
| MOTA | 2230 | CB ASN A 280 | 54.724 | | 1.00 23.68 |
| MOTA | 2231 | CG ASN A 280 | 55.508 | | 1.00 34.47 |
| MOTA | 2232 | OD1 ASN A 280 | 54.958 56.809 | | 1.00 33.59 |
| MOTA | 2233 | | 52.493 | | 1.00 30.46 |
| MOTA | 2234 | | 51.899 | 23.182 125.677 | 1.00 27.66 |
| ATOM | 2235 | | 52.429 | 22.960 123.509 | 1.00 27.32 |
| ATOM | 2236 | | 51.620 | 24.107 123.128 | 1.00 31.07 |
| ATOM | 2237 | | 51.878 | 24.517 121.666 | 1.00 35.08 |
| MOTA | 2238 2239 | | 50.776 | 25.445 121.174 | 1.00 34.33 |
| ATOM | 2240 | | 53.253 | 25.185 121.562 | 1.00 33.53 |
| ATOM | 2240 | | 53.590 | 25.694 120.178 | 1.00 34.88 |
| ATOM ATOM | 2242 | C ILE A 281 | 50.141 | | 1.00 31.22 1.00 30.15 |
| ATOM | 2243 | 0 ILE A 281 | 49.391 | | |
| ATOM | 2244 | | 49.723 | 22.606 122.923 | 1.00 30.91 |
| 71. | | | | | |

| | | - | 8 |
|-------|------|-------------------------------|--|
| : | 2245 | CA VAL A 282 | 48.332 22.214 123.081 1.00 30.76 |
| MOTA | 2245 | | 49 075 20 707 122.523 1.00 35.10 |
| MOTA | 2246 | CB VAL A 282 CG1 VAL A 282 | 46 641 20 358 122.841 1.00 28.72 |
| ATOM | 2247 | | 48 313 20 781 121.018 1.00 28.66 |
| MOTA | 2248 | CG2 VAL A 282 | 47 952 22 236 124.558 1.00 31.39 |
| ATCM | 2249 | C VAL A 282 | 46 884 22 715 124.917 1.00 32.70 |
| MOTA | 2250 | O VAL A 282 | 48.837 21.720 125.406 1.00 29.86 |
| MOTA' | 2251 | N ARG A 283 | 48.587 21.675 126.840 1.00 34.82 |
| MOTA | 2252 | CA ARG A 283 | 49.629 20.785 127.519 1.00 31.44 |
| MOTA | 2253 | CB ARG A 283 | 49.551 19.334 127.061 1.00 29.49 |
| MOTA | 2254 | CG- ARG A 283 | 50.729 18.539 127.554 1.00 30.67 |
| ATOM | 2255 | CD ARG A 283 | 50.730 18.314 128.990 1.00 30.78 |
| MOTA | 2256 | NE ARG A 283 | 51.826 18.351 129.742 1.00 35.27 |
| ATOM | 2257 | CZ ARG A 283 | 53.012 18.611 129.198 1.00 36.46 |
| MOTA | 2258 | NH1 ARG A 283 | 51.742 18.100 131.035 1.00 35.90 |
| ATOM | 2259 | NH2 ARG A 283 | 48.561 23.065 127.473 1.00 36.06 |
| ATOM | 2260 | C ARG A 283 | 47.830 23.302 128.439 1.00 35.04 |
| MOTA | 2261 | O ARG A 283 | 49.350 23.985 126.928 1.00 35.70 |
| MOTA | 2262 | N GLU A 284 | 49.376 25.348 127.448 1.00 40.93 |
| ATOM | 2263 | CA GLU A 284 | 50.499 26.166 126.799 1.00 44.17 |
| ATOM | 2264 | CB GLU A 284 | 51.917 25.702 127.141 1.00 56.39 |
| MOTA | 2265 | CG GLU A 284 | 52.989 26.495 126.401 1.00 60.69 |
| MOTA | 2266 | CD GLU A 284 | 53.012 27.738 126.542 1.00 63.13 |
| MOTA | 2267 | OE1 GLU A 284 | 53.810 25.880 125.680 1.00 62.79 |
| MOTA | 2268 | OE2 GLU A 284 | 33.010 23.000 100 100 30 34 |
| ATOM | 2269 | C GLU A 284 | 40.000 20.000 00 00 50 |
| ATOM | 2270 | O GLU A 284 | 47.525 26.783 127.954 1.00 38.32 47.472 25.704 125.986 1.00 33.75 |
| MOTA | 2271 | N VAL A 285 | 4/.4/2 23./3 100 100 25 02 |
| ATOM | 2272 | CA VAL A 285 | 46.205 26.294 125.592 1.00 35.82 46.039 26.291 124.062 1.00 34.14 |
| MOTA | 2273 | CB VAL A 285 | 44.654 26.811 123.693 1.00 36.43 |
| ATOM | 2274 | CG1 VAL A 285 | 44.034 20.033 1.00 1.00 37 36 |
| MOTA | 2275 | CG2 VAL A 285 | 47.114 27.153 123.419 1.00 37.20 44.964 25.638 126.192 1.00 38.96 |
| ATOM | 2276 | C VAL A 285 | 44.043 26.336 126.611 1.00 41.83 |
| ATOM | 2277 | O VAL A 285 | 44.931 24.308 126.236 1.00 37.57 |
| MOTA | 2278 | N PHE A 286 | 43.760 23.608 126.753 1.00 35.05 |
| MOTA | 2279 | CA PHE A 286 | 43.159 22.723 125.657 1.00 32.53 |
| ATOM | 2280 | CB PHE A 286 | 42.544 23.490 124.529 1.00 30.15 |
| ATOM | 2281 | CG PHE À 286 | 43 104 23 459 123,256 1.00 33.96 |
| ATOM | 2282 | CD1 PHE A 286 | 41 308 24 245 124.736 1.00 30.30 |
| MOTA | 2283 | CD2 PHE A 286 | 42.527 24.170 122.202 1.00 32.96 |
| MOTA | 2284 | CE1 PHE A 286 | 40 813 24 958 123.693 1.00 31.67 |
| MOTA | 2285 | CE2 PHE A 286 | λ_1 301 24 919 122.419 1.00 31.66 |
| ATOM | 2286 | CZ PHE A 286 | 42 922 22 773 128,015 1.00 35.18 |
| MOTA | 2287 | C PHE A 286 | 42 984 22 080 128,409 1.00 36.97 |
| MOTA | 2288 | O PHE A 286 | 45 096 22 840 128,656 1.00 30.8/ |
| ATOM | 2289 | N GLY A 287 | 45 207 22 056 129.862 1.00 30.06 |
| ATCM | 2290 | CA GLY : 287 | 45 525 20 590 129.527 1.00 34.44 |
| MOTA | 2291 | C GLY 1. 287 | 45.914 20.264 128.403 1.00 32.54 |
| ATOM | 2292 | O GLY 7. 287 | 45 200 10 710 130.500 1.00 28.42 |
| MOTA | 2293 | N GLU A 288 | 45 464 18 273 130.310 1.00 32.23 |
| MOTA | 2294 | CA GLU A 288 | 45 613 17 576 131 663 1.00 37.02 |
| ATOM | 2295 | CB GLU A 288 | 46.910 17.864 132.411 1.00 45.36 |
| ATCM | 2296 | CG GLU A 288 | 48.140 17.455 131.622 1.00 45.65 |
| ATOM | 2297 | | 40 144 16 334 131 069 1.00 46 42 |
| ATCM | 2298 | OE1 GLU A 288 | 40.144 10.334 507 1 00 50 78 |
| MOTA | 2299 | | 49.106 18.245 131.571 1.00 30.78 44.309 17.623 129.546 1.00 30.98 |
| MOTA | 2300 | C GLU A 288 | 44.303 1,00 29 67 |
| ATOM | 2301 | | 44 641 16 694 128 657 1.00 29.66 |
| ATOM | 2302 | N GLY A 289 | 19.041 |
| ATCM | 2303 | CA GLY A 289 | 43.023 43.333 == 4.00 30 45 |
| ATCM | 2304 | C GLY A 289 | 14 518 14 207 128 739 1.00 25.90 |
| ATCM | 2305 | 5 O GLY A 289 | 42 384 13 807 126 868 1.00 26.21 |
| ATOM | 2306 | N VAL A 290 | 13.504 13.503 126.718 1.00 27.31 |
| ATOM | 2307 | 7 CA VAL A 290 | 42 200 11 626 126,412 1.00 26.53 |
| ATOM | 2308 | 3 CB VAL A 290 | 12.554 10.149 126.204 1.00 25.36 |
| ATCM | 2309 |) CG1 VAL A 290 | 42.334 10.110 107 565 1 00 24 38 |
| 2 TOM | | | 41.308 11.822 127.565 1.00 24.38 |

| | 771 | A 290 | 44.580 | 12.248 | 125.550 | 1.00 24.52 |
|-------|--------------|-----------|---------|---------|-----------|--------------|
| ATOM | | | 44.307 | 12.743 | 124 461 | 1.00 26.84 |
| ATOM | 2312 O VAL | A 290 | 44.307 | 12.743 | | 1.00 23.56 |
| ATOM | 2313 N TYR | A 291 | 45.716 | 11.597 | 125.775 | 1.00 23.30 |
| | | A 291 | 46.729 | 11.478 | 124.732 | 1.00 23.74 |
| ATOM | | | 48.092 | 11.817 | 125.342 | 1.00 18.40 |
| ATOM | | A 291 | 40.022 | 13.113 | 126 118 | 1.00 21.60 |
| ATOM | 2316 CG TYR | A 291 | 48.040 | 13.113 | 120.110 | 1.00 23.83 |
| | 2317 CD1 TYR | A 291 | 48.326 | 13.148 | 127.483 | 1.00 23.03 |
| ATOM | | 3 291 | 48.200 | 14.331 | 128.214 | 1.00 24.57 |
| ATOM | | 201 | 47.634 | 14.291 | 125.503 | 1.00 18.17 |
| ATOM | 2319 CD2 TYR | A 291 | | 15 476 | 126.220 | 1.00 26.36 |
| ATOM | 2320 CE2 TYR | A 291 | 47.504 | | | 1.00 27.68 |
| | | A 291 | 47.786 | | 127.575 | 1.00 27.00 |
| ATOM | | A 291 | 47.631 | | 128.283 | 1.00 28.92 |
| ATOM | • | . A 231 | 46.768 | 10 118 | 124.044 | 1.00 23.03 |
| ATOM | 2323 C TYR | A 291 | 46.700 | 0.110 | 124.707 | 1.00 20.66 |
| | 2324 O TYR | A 291 | 46.837 | | 124.707 | 1.00 23.96 |
| ATOM | | A 292 | 46.755 | 10.142 | 122.711 | 1.00 23.90 |
| ATOM | | | 46.767 | 8.924 | 121.902 | 1.00 20.69 |
| ATOM | 2326 CA LEU | A 292 | | 8.842 | 121.076 | 1.00 22.13 |
| ATOM | 2327 CB LEU | A 292 | 45.482 | | 121.814 | 1.00 23.78 |
| | 2328 CG LEU | J A 292 | 44.162 | | | 1 00 23 09 |
| ATOM | | J A 292 | 43.001 | 8.959 | 120.826 | 1.00 23.09 |
| ATOM | | . 200 | 44.008 | 8.050 | 122.930 | 1.00 16.01 |
| ATOM | 2330 CD2 LEU | J A 292 | | 0 095 | 120.947 | 1.00 22.90 |
| ATOM | 2331 C LEU | J A 292 | 47.953 | 0.005 | 120.517 | 1.00 22.31 |
| | 2332 O LEU | J A 292 | 48.527 | 9.923 | 120.617 | |
| ATOM | | A 293 | 48.301 | 7.684 | 120.491 | 1.00 18.83 |
| ATOM | | A 433 | 49.401 | 7 529 | 119.554 | 1.00 24.35 |
| ATOM | 2334 CA GL | 7 A 293 | | 7.046 | 118.154 | 1.00 24.22 |
| | 2335 C GL | Y A 293 | 48.908 | 7.840 | 110.134 | 1.00 20.46 |
| MOTA | | Y A 293 | 48.025 | 8.684 | 117.991 | 1.00 20.40 |
| ATOM | | Y A 294 | 49.459 | 7.177 | 117.148 | 1.00 24.63 |
| ATOM | | Y A 294 | 49.035 | 7 423 | 115.779 | 1.00 22.03 |
| ATOM | 2338 CA GL | Y A 294 | | 7.423 | 114.769 | 1.00 22.90 |
| ATOM | 2339 C GL | Y A 294 | 50.024 | 6.869 | 114.703 | 1.00 24.10 |
| | | Y A 294 | 50.956 | 6.150 | 115.136 | 1.00 24.10 |
| MOTA | | | 49.825 | 7,203 | 113.499 | 1.00 19.85 |
| ATOM | | Y A 295 | | 6 724 | 112.458 | 1.00 23.33 |
| MOTA | 2342 CA GL | Y A 295 | 50.721 | 7.723 | 112.740 | 1.00 19.01 |
| | 2343 C GL | Y A 295 | 52.185 | 7.010 | 112.790 | |
| ATOM | | Y A 295 . | 52.541 | 8.094 | 113.196 | 1.00 19.39 |
| ATOM | | I A 200 . | 53.035 | 6.026 | 112.472 | 1.00 25.85 |
| ATOM | 2345 N GL | Y A 296 | | 6 162 | 112.690 | 1.00 22.65 |
| ATOM | 2346 CA GL | Y A 296 | 54.468 | 0.102 | 112.000 | 1.00 25.31 |
| | 2347 C' GL | Y A 296 | 55.098 | 4.898 | 112.146 | 1.00 25.52 |
| ATOM | | Y A 296 | 54.778 | 3.798 | 112.609 | 1.00 25.86 |
| ATOM | | 1 A 250 | 56.005 | 5.034 | 111.185 | 1.00 22.83 |
| ATOM | 2349 N TY | R A 297 | | 3 052 | 110.577 | 1.00 23.93 |
| ATOM | 2350 CA TY | R A 297 | 56.598 | 3.652 | 100.37 | 1.00 21.59 |
| | 2351 CB TY | R A 297 | 56.137 | 3.780 | 109.125 | 1.00 21.35 |
| ATOM | | R A 297 | 54.660 | 4.084 | 109.035 | 1.00 25.85 |
| ATOM | | K A 237 | 54.203 | 5 402 | 109.017 | 1.00 22.28 |
| ATOM | 2353 CD1 TY | R A 297 | 54.203 | | 109.089 | 1.00 20.19 |
| ATOM | 2354 CE1 TY | R A 297 | 52.842 | | | |
| | 2355 CD2 TY | R A 297 | 53.713 | 3.062 | 109.116 | |
| ATOM | | R A 297 | 52.352 | 3.346 | 5 109.190 | 1.00 21.83 |
| ATOM | | K A 231 | 51.927 | | 5 109.181 | 1.00 21.81 |
| ATOM | 2357 CZ TY | R A 297 | | | 2 109.305 | |
| ATOM | 2358 OH TY | R A 297 | 50.588 | | 4 110 674 | |
| | 2359 C TY | r a 297 | 58.104 | | 4 110.674 | |
| ATOM | | R A 297 | 58.665 | 2.72 | 4 110.154 | 1.00 22.07 |
| -TOM | | CR A 497 | 58.765 | | | 1.00 23.71 |
| ATOM | 2361 N H | IS A 298 | | | | |
| | 2362 CA HI | IS A 298 | 60.204 | 4.53 | | |
| ATOM | | IS A 298 | 60.913 | 5.85 | | |
| ATOM | | TO 2 200 | 62.403 | 5.72 | 7 111.213 | 1.00 33.08 |
| ATOM | 2364 CG H | IS A 298 | 62.302 | | | 1.00 31.83 |
| ATOM | 2365 CD2 H | IS A 298 | 63.273 | | | |
| | | IS A 298 | 63.151 | 5.77 | | |
| ATOM | | 10 3 200 | 64.419 | 5.54 | | |
| ∴TOM | 2367 CE1 H | IS A 298 | 64.520 | | | 3 1.00 38.70 |
| -TCM | 2368 NE2 H | IS A 298 | 04. 141 | | | |
| | | IS A 298 | 60.37 | 4.18 | | |
| ATOM | | IS A 298 | 60.120 | 5.02 | 0 113.865 | |
| ATOM | | 10 : 200 | 60.82 | 9 2.96 | 3 113.29 | 1.00 29.37 |
| - TOM | | RO A 299 | 61.28 | | 2 112.35 | 1.00 26.09 |
| ATOM | i 2372 CD P | RO A 299 | 01.48 | | 1 114.66 | |
| | | RO A 299 | 61.02 | | . 114 47 | |
| ATOM | | RO A 299 | 61.67 | | 8 114 46 | |
| 10T £ | | 20 7 200 | 62.41 | 1 1.30 | 6 113.13 | 7 1.00 27.34 |
| - TCN | 1 2375 CG P | RO A 299 | 61.84 | | 3 115.57 | 0 1.00 31.88 |
| -701 | 1 2376 C P | RO A 299 | 61.54 | ٠ ٠ ٠٠٠ | , | |
| | | | | | | |

| | • | | 6 | | |
|--------------|--------------|-------------------------------|------------------|---------------------------------|--------------------------|
| > mOM | 2377 | O PRO A 299 | 61.480 | | 1.00 32.45 |
| MOTA MOTA | 2378 | N TYR A 300 | 62.959 | | 1.00 27.41 |
| ATOM | 2379 | CA TYR A 300 | 63.803 | 4.007 775. | 1.00 27.34 1.00 26.84 |
| ATOM | 2380 | CB TYR A 300 | 65.163 | | |
| MOTA | 2381 | CG TYR A 300 | 65.912 | | 1.00 29.09 1.00 30.93 |
| ATOM | 2382 | CD1 TYR A 300 | 65.517 | | 1.00 30.93 |
| ATOM | 2383 | CE1 TYR A 300 | 66.214 | 1.411 114.682 | 1.00 30.88 |
| ATOM | 2384 | CD2 TYR A 300 | 67.027 | 3.941 113.908 | 1.00 29.72 |
| ATOM | 2385 | CE2 TYR A 300 | 67.730 | 2.829 113.466 | 1.00 33.89 |
| MOTA | 2386 | CZ TYR A 300 | 67.320 | 1.568 113.854 | 1.00 34.70 |
| ATOM | 2387 | OH TYR A 300 | 68.011 | 0.471 113.404 | 1.00 23.44 |
| ATOM | 2388 | C TYR A 300 | 63.113 | 6.134 116.137 6.631 117.264 | 1.00 23.87 |
| ATOM | 2389 | O TYR A 300 | 63.108 | 6.711 115.092 | 1.00 22.19 |
| ATOM | 2390 | N ALA A 301 | 62.530 | 7.993 115.216 | 1.00 26.50 |
| ATOM | 2391 | CA ALA A 301 | 61.839 61.266 | 8.416 113.864 | 1.00 24.16 |
| MOTA | 2392 | CB ALA A 301 | 60.715 | 7.878 116.237 | 1.00 27.86 |
| MOTA | 2393 | C ALA A 301 | 60.556 | 8.728 117.117 | 1.00 22.47 |
| MOTA | 2394 | O ALA A 301 | 59.940 | 6.808 116.110 | 1.00 23.27 |
| MOTA | 2395 | N LEU A 302 | 58.818 | 6.566 116.996 | 1.00 26.50 |
| MOTA | 2396 | CA LEU A 302 CB LEU A 302 | 58.036 | 5.354 116.483 | 1.00 26.02 |
| MOTA | 2397 | | 56.866 | 4.798 117.291 | 1.00 29.73 |
| MOTA | 2398 | CG LEU A 302 CD1 LEU A 302 | 55.983 | 3.938 116.394 | 1.00 31.01 |
| ATOM | 2399 | CD2 LEU A 302 | 57.394 | 4.001 118.465 | 1.00 32.99 |
| MOTA | 2400 2401 | C LEU A 302 | 59.246 | 6.373 118.451 | 1.00 27.49 |
| MOTA | 2402 | O LEU A 302 | 58.648 | 6.946 119.358 | 1.00 25.22 1.00 27.85 |
| MOTA MOTA | 2403 | N ALA A 303 | 60.289 | 5.580 118.672 | 1.00 27.83 |
| ATOM | 2404 | CA ALA A 303 | 60.765 | 5.320 120.024 | 1.00 27.33 |
| ATOM | 2405 | CB ALA A 303 | 61.854 | 4.269 119.990 6.580 120.714 | 1.00 26.64 |
| ATOM | 2406 | C ALA A 303 | 61.279 | 6.849 121.875 | 1.00 23.18 |
| ATOM | 2407 | O ALA A 303 | 60.944 | 7.354 120.003 | 1.00 27.48 |
| ATOM | 2408 | N ARG A 304 | 62.092 | 8.570 120.581 | 1.00 25.46 |
| MOTA | 2409 | CA ARG A 304 | 62.648 63.773 | 9.136 119.704 | 1.00 21.31 |
| MOTA | 2410 | CB ARG A 304 CG ARG A 304 | 65.005 | 8.231 119.562 | 1.00 25.98 |
| MOTA | 2411 | | 66.153 | 9.042 118.951 | 1.00 27.87 |
| MOTA | 2412 | - ^ ^ | 65.647 | 9.766 117.796 | 1.00 36.76 |
| ATOM | 2413 2414 | NE ARG A 304 CZ ARG A 304 | 66.207 | 10.838 117.261 | 1.00 30.79 |
| MOTA | 2414 | NH1 ARG A 304 | 67.323 | 11.345 117.768 | 1.00 30.11 |
| MOTA | 2416 | NH2 ARG A 304 | 65.623 | 11.419 116.225 | 1.00 36.07 1.00 25.46 |
| MOTA MOTA | 2417 | C ARG A 304 | 61.585 | 9.634 120.803 | 1.00 24.23 |
| ATOM | 2418 | O ARG A 304 | 61.519 | 10.237 121.876 | 1.00 22.22 |
| ATOM | 2419 | N ALA A 305 | 60.741 | 9.854 119.802 10.868 119.910 | 1.00 26.70 |
| ATOM | 2420 | CA ALA A 305 | 59.700 | 10.868 119.910 | 1.00 28.14 |
| ATOM | 2421 | CB ALA A 305 | 58.914 | 10.626 121.072 | 1.00 25.54 |
| MOTA | 2422 | | 58.749 58 513 | 11.520 121.883 | 1.00 24.1/ |
| MOTA | 2423 | | 58 1.89 | 9.426 121.160 | 1.00 25.66 |
| MOTA | 2424 | | 57.270 | 9.157 122.253 | 1.00 28.01 |
| MOTA | 3425 | | 56.454 | 7.873 122.012 | 1.00 18.66 |
| MOTA | 2426 | | 55.382 | 8.052 120.973 | 1.00 21.80 |
| MOTA | 2427 | | 54.709 | 7.019 120.240 | 1.00 24.88 |
| MOTA | 2428 2429 | | 53.725 | 7.646 119.442 | 1.00 23.98 |
| MOTA | 2430 | | 54.839 | 5.623 120.181 | 1.00 23.26 1.00 20.24 |
| MOTA | 2431 | | 54.795 | 9.228 120.599 | |
| MOTA MOTA | 2432 | 36/ | 53.799 | 8.995 119.681 | |
| MOTA | 2433 | | 52.875 | 6.926 118.590 | |
| ATOM | 2434 | CZ3 TRP A 306 | 53.993 | 4.906 119.335 5.562 118.550 | |
| ATOM | 2435 | CH2 TRP A 306 | 53.024 | | |
| ATOM | 2436 | C TRP A 306 | 57.969 | 9.113 123.605 9.319 124.637 | |
| ATOM | 2431 | 7 O TRP A 306 | 57.330 | 8.851 123.615 | 1.00 26.76 |
| ATOM | 2438 | 3 N THR A 307 | 59.273 | 8.850 124.881 | 1.00 22.81 |
| ATOM | 2439 | CA THR A 307 | 60.000 61.457 | 8.319 124.730 | 1.00 25.54 |
| MOTA | 244 | | | 6 902 124.504 | 1.00 22.73 |
| ATOM | 244 | | | - 405 000 | |
| MOTA | - 4 4 1 | 2 CG2 THR A 307 | 04.203 | J | |

| | | > 207 | 60.027 | 10.288 125.396 | 1.00 26.54 |
|-------|------|---------------|----------|----------------|--------------|
| MOTA | 2443 | C THR A 307 | | 10.526 126.604 | 1.00 25.34 |
| MOTA | 2444 | O THR A 307 | | 11.247 124.478 | 1.00 21.65 |
| ATOM | 2445 | N LEU A 308 | | | 1.00 21.41 |
| ATOM | 2446 | CA LEU A 308 | | 12.03. 20 | 1.00 19.20 |
| ATOM | 2447 | CB LEU A 308 | | 13.330 220 | 1.00 21.31 |
| ATOM | 2448 | CG LEU A 308 | | 13.386 122.938 | 1.00 21.31 |
| | 2449 | CD1_LEU A 308 | 61.900 | 14.362 121.774 | 1.00 21.75 |
| ATOM | | CD2 LEU A 308 | 62.937 | 13.622 123.915 | 1.00 19.26 |
| MOTA | 2450 | | 58 811 | 12.981 125.479 | 1.00 25.18 |
| MOTA | 2451 | | 58.731 | 13.565 126.561 | 1.00 21.35 |
| MOTA | 2452 | O LEU A 308 | . 57.743 | 12.567 124.806 | 1.00 21.74 |
| MOTA | 2453 | N ILE A 309 | 56.394 | 12.799 125.298 | 1.00 19.23 |
| MOTA | 2454 | CA ILE A 309 | | 12.149 124.366 | 1.00 19.63 |
| MOTA | 2455 | CB ILE A 309 | | 12.321 124.948 | 1.00 19.54 |
| MOTA | 2456 | CG2 ILE A 309 | 53.945 | | 1.00 20.80 |
| MOTA | 2457 | CG1 ILE A 309 | 55.403 | 12.788 122.979 | 1.00 20.08 |
| ATOM | 2458 | CD1 ILE A 309 | 55.118 | 14.274 122.988 | 1.00 23.97 |
| MOTA | 2459 | C ILE A 309 | 56.228 | 12.222 126.701 | 1.00 23.37 |
| | 2460 | O ILE A 309 | 55.731 | 12.894 127.602 | |
| ATOM | 2461 | N TRP A 310 | 56.652 | 10.977 126.888 | 1.00 26.45 |
| MOTA | 2462 | CA TRP A 310 | 56.525 | 10.342 128.192 | 1.00 28.35 |
| MOTA | | | 56.940 | 8.872 128.132 | 1.00 23.95 |
| MOTA | 2463 | | 56.874 | 8.203 129.479 | 1.00 29.60 |
| MOTA | 2464 | CG TRP A 310 | 551.697 | 7.967 130.263 | 1.00 31.40 |
| MOTA | 2465 | CD2 TRP A 310 | 56.115 | 7.390 131.480 | 1.00 32.47 |
| ATOM. | 2466 | CE2 TRP A 310 | | 8.189 130.055 | 1.00 32.30 |
| MOTA | 2467 | CE3 TRP A 310 | 54.329 | 7.770 130.232 | 1.00 33.42 |
| ATOM | 2468 | CD1 TRP A 310 | 57.926 | 7.282 131.436 | 1.00 30.09 |
| MOTA | 2469 | NE1 TRP A 310 | 57.480 | 7.030 132.492 | 1.00 29.93 |
| ATOM | 2470 | CZ2 TRP A 310 | 55.213 | 7.030 132.432 | 1.00 29.72 |
| ATOM | 2471 | CZ3 TRP A 310 | 53.432 | 7.831 131.062 | 1.00 24.53 |
| ATOM | 2472 | CH2 TRP A 310 | 53.881 | 7.259 132.265 | 1.00 24.33 |
| | 2473 | C TRP A 310 | 57.308 | 11.048 129.293 | 1.00 33.43 |
| MOTA | 2474 | O TRP A 310 | 56.820 | 11.137 130.426 | 1.00 27.59 |
| ATOM | 2475 | N CYS A 311 | 58.512 | 11.535 128.984 | 1.00 29.34 |
| ATOM | | | 59.305 | 12.247 129.994 | 1.00 30.06 |
| MOTA | 2476 | | 60.722 | 12.538 129.479 | 1.00 30.08 |
| MOTA | 2477 | | 61.804 | 11.084 129.327 | 1.00 33.17 |
| MOTA | 2478 | | 58.612 | 13.560 130.397 | 1.00 29.25 |
| MOTA | 2479 | C CYS A 311 | 58.612 | 13.940 131.570 | 1.00 28.80 |
| MOTA | 2480 | O CYS A 311 | 58.021 | 14.247 129.425 | 1.00 23.13 |
| MOTA | 2481 | N GLU A 312 | 57.308 | 15.496 129.696 | 1.00 30.31 |
| ATOM | 2482 | CA GLU A 312 | | 16.032 128.427 | 1.00 28.97 |
| ATOM | 2483 | CB GLU A 312 | 56.648 | 17.418 127.988 | 1.00 41.67 |
| ATOM | 2484 | CG GLU A 312 | 57.080 | 18.465 129.059 | 1.00 44.21 |
| MOTA | 2485 | CD GLU A 312 | 56.905 | 18.534 129.658 | 1.00 54.15 |
| ATOM | 2486 | OE1 GLU A 312 | 55.813 | 18.534 129.030 | 1.00 43.90 |
| ATOM | 2487 | OE2 GLU A 312 | 57.860 | 19.233 129.290 | 1.00 28.03 |
| ATOM | 2488 | C GLU A 312 | 56.204 | 15.225 130.712 | 1.00 30.64 |
| | 2489 | 10 | 56.120 | 15.869 131.751 | 1.00 30.04 |
| MOTA | 2490 | 010 | 55.343 | 14.270 130.388 | 1.00 31.06 |
| MOTA | | | 54.231 | 13.918 131.266 | 1.00 36.21 |
| MOTA | 2491 | | 53.337 | 12.873 130.604 | 1.00 28.83 |
| MOTA | 2492 | | 52.493 | 13.342 129.429 | 1.00 34.62 |
| MOTA | 2493 | | 51.818 | 12,146 128.788 | 1.00 33.05 |
| MOTA | 2494 | | 51.471 | 14.357 129.914 | 1.00 27.27 |
| ATOM | 2495 | | | 13.377 132.610 | 1.00 33.97 |
| MOTA | 2496 | | 54.685 | 13.730 133.644 | |
| ATOM | 2497 | O LEU A 313 | 54.131 | 12.508 132.577 | |
| ATOM | 2498 | N SER A 314 | 55.688 | 11.880 133.776 | |
| MOTA | 2499 | CA SER A 314 | 56.233 | | |
| | 2500 | | 57.183 | | |
| ATOM | 2501 | | 56.517 | 9.761 132.628 | |
| MOTA | 2502 | | 57.002 | | |
| ATOM | | | 57.339 | 12.513 135.788 | 1.00 27.69 |
| ATOM | 2503 | | 57.312 | 14.021 134.130 | 1.00 35.50 |
| ATOM | 2504 | | 58.057 | 14 996 134 905 | 1.00 36.31 |
| atom | 2505 | | 59.518 | 14.634 135.099 | 1.00 38.47 |
| ATOM | 2500 | | 60.138 | 15.049 136.078 | 3 1.00 41.5/ |
| ATOM | 250 | | 60.089 | | 1.00 39.32 |
| ATCM | 250 | 8 N ARG A 316 | 60.009 | 10.00 | |

| | | | | | | 12 501 | 134.332 | 1.00 3 | 9.06 |
|------|--------|-------|---------------|---------|--------|---------|-----------|--------|----------------|
| MOTA | 2509 | CA · | ARG A | 316 | 61.490 | | | 1.00 3 | |
| ATOM | 2510 | CB A | ARG A | 316 | 61.641 | | 134.413 | 1.00 3 | 9.10 |
| | | | ARG A | | 61.233 | 11.226 | 133.184 | 1.00 3 | |
| MOTA | 2511 | | | | 61.426 | | 133.429 | 1.00 4 | 1.21 |
| MOTA | 2512 | | ARG A | | | | 134.389 | 1.00 4 | |
| ATOM | 2513 | | ARG A | | 60.461 | 9.229 | 134.305 | 1.00 | |
| ATOM | 2514 | CZ . | ARG A | 316 | 60.524 | | 134.926 | | |
| | | | ARG A | | 61.511 | 7.209 | 134.598 | 1.00 3 | |
| AŤOM | 2515 | | | | 59.583 | 7.621 | 135.768 | 1.00 3 | 30.53 |
| ATOM | 2516 | | ARG A | | _ | | 133.230 | 1.00 4 | |
| ATOM | 2517 | С | ARG A | 316 | 62.369 | 14.083 | | 1.00 | |
| ATOM | 2518 | 0 - | ARG A | 316 | 61.910 | 14.325 | 132.111 | | |
| | | | GLU A | | 63.633 | 14.325 | 133.564 | 1.00 4 | 11.26 |
| MOTA | 2519 | N | GLU A | 217 | 64.580 | 14.905 | 132.619 | 1.00 4 | 14.42 |
| ATOM | 2520 | CA | GLU A | 31/ | | | 133.317 | 1.00 4 | |
| ATOM | 2521 | CB | GLU A | 317 | 65.901 | 15.249 | 133.317 | | 57.66 |
| | 2522 | CG | GLU A | 317 | 65.756 | 15.996 | 134.629 | | |
| MOTA | | CD | GLU A | 317 | 65.212 | 15.113 | 135.743 | 1.00 | |
| ATOM | 2523 | | | | 65.871 | 14.101 | 136.073 | 1.00 | 6 8 .38 |
| MOTA | 2524 | OE1 | GLU A | 31/ | 64 120 | | 136.287 | 1.00 | |
| MOTA | 2525 | OE2 | GLU A | 317 | 64.129 | | | 1.00 | |
| ATOM | 2526 | С | GLU A | 317 | 64.873 | | 131.462 | | |
| | | ō | GLU A | | 64.977 | 12.748 | 131.636 | 1.00 | 38.84 |
| MOTA | 2527 | | | | 65.010 | 14 525 | 130.275 | 1.00 | 37.64 |
| ATOM | 2528 | N | VAL A | | | 112 720 | 129.108 | 1.00 | 39.13 |
| MOTA | 2529 | CA | VAL A | | 65.315 | 13.720 | 127.100 | 1.00 | |
| ATOM | 2530 | CB | VAL A | 318 | 64.858 | 14.417 | 127.810 | | |
| | | | VAL A | | 65.192 | 13.544 | 126.610 | 1.00 | |
| MOTA | 2531 | CGI | VALA | 710 | 63.364 | 14 701 | 127.867 | 1.00 | 42.38 |
| ATOM | 2532 | | VAL A | 210 | | 13.495 | | | 38.45 |
| MOTA | 2533 | С | VAL A | 318 | 66.822 | 13.433 | | | 36.04 |
| ATOM | 2534 | 0 | VAL A | 318 | 67.598 | 14.442 | 128.910 | | |
| | | N | | 319 | 67.261 | 12.236 | 129.156 | | 39.54 |
| ATOM | 2535 | | | | 66.512 | 10 994 | 129.397 | 1.00 | 40.47 |
| ATOM | 2536 | CD | PRO A | | | 11 0/0 | 129.088 | 1.00 | 43.85 |
| ATOM | 2537 | CA | PRO A | 319 | 68.695 | 11.343 | 120.000 | | 44.12 |
| MOTA | 2538 | CB | PRO A | 319 . | 68.745 | 10.439 | 129.319 | | |
| | 2539 | CG | PRO A | | 67.419 | 9.986 | 128.745 | | 46.48 |
| MOTA | | | PRO A | | 69.228 | 12.353 | 127.718 | | 43.55 |
| MOTA | 2540 | C | | | | 12 141 | 126.708 | 1.00 | 43.45 |
| ATOM | 2541 | 0 | PRO A | | 68.563 | 12.141 | 127.689 | | 42.52 |
| ATOM | 2542 | N | GLU A | 320 | 70.420 | 12.930 | 127.009 | | 45.19 |
| | 2543 | CA | GLU A | | 71.026 | 13.380 | 126.440 | | |
| MOTA | | | GLU A | | 72.384 | 14.032 | 126.706 | 1.00 | 43.86 |
| MOTA | 2544 | СВ | | | 73.121 | 14 412 | 125.434 | 1.00 | 52.62 |
| ATOM | 2545 | CG | GLU A | | | 14 067 | 125.697 | 1 00 | 52.36 |
| ATOM | 2546 | CD | GLU A | | 74.507 | 14.907 | 123.037 | 1 00 | 56.25 |
| MOTA | 2547 | OEl | GLU A | 320 | 75.219 | 15.271 | 124.720 | | |
| | | OE2 | GLU A | 320 | 74.883 | 15.101 | 126.875 | | 52.25 |
| ATOM | . 2548 | | GLU A | 220 | 71.223 | 12.266 | 125.421 | 1.00 | 43.52 |
| MOTA | 2549 | С | GLU A | | | 12 /12 | 124.253 | 1.00 | 41.89 |
| MOTA | 2550 | 0 | GLU A | | 70.876 | 12.412 | 124.223 | | 43.35 |
| ATOM | 2551 | N | LYS A | 321 | 71.781 | 11.150 | 125.867 | | |
| | | CA | LYS A | | 72.059 | 10.041 | 124.969 | | 43.53 |
| MOTA | 2552 | | DIS :: | 221 | 73.561 | 9.808 | 124.879 | 1.00 | 42.78 |
| ATOM | 2553 | CB | LYS A | | | 0 340 | 126.180 | 1.00 | 49.38 |
| MOTA | 2554 | CG | LYS A | | 74.238 | | | 1 00 | 57.82 |
| ATOM | 2555 | CD | LYS A | 321 | 74.272 | 10.396 | , 127.307 | 1.00 | 53.81 |
| | 2556 | CE | LYS A | 321 | 72.978 | 10.497 | 128.129 | 1.00 | 33.61 |
| MOTA | | | LYS A | 321 | 72.660 | 9.24 | 128.883 | 1.00 | 54.17 |
| ATOM | 2557 | NZ | LIS A | 321 | 71.407 | 8 73 | 125.345 | 1.00 | 41.52 |
| ATOM | 2558 | С | LYS A | . 321 | | 0.73. | 126.469 | 1 00 | 41.98 |
| MOTA | 2559 | 0 | LYS A | 321 | 70.954 | 8.54 | 120.405 | 1.00 | 38.64 |
| ATOM | 2560 | N | LEU A | 322 | 71.378 | 7.820 | 124.382 | 1.00 | 30.04 |
| | 2560 | CA | LEU A | 322 | 70.815 | 6.50 | 3 124.613 | 1.00 | 40.46 |
| MOTA | 2561 | | | | 70.442 | 5 84 | 5 123.289 | 1.00 | 42.22 |
| MOTA | 2562 | CB | LEU A | 322 | | 6 63 | 2 122.287 | 1.00 | 42.92 |
| MOTA | 2563 | CG | LEU A | 322 | 69.595 | 0.03. | 2 122.207 | 1.00 | 41.13 |
| | 2564 | כתו | LEU A | 322 | 69.204 | 5.73 | 7 121.125 | 1.00 | 44.44 |
| MOTA | | 201 | LEU A | 322 | 68.361 | 7.14 | 8 122.967 | 1.00 | 44.41 |
| MOTA | 256.5 | | , <u></u> u A | 200 | 71.918 | 5 70 | 2 125.268 | 1.00 | 41.36 |
| MOTA | 2566 | С | LEU A | 322 | | 5.70 | 5 124.884 | 1 00 | 44.16 |
| ATOM | 2567 | 0 | LEU A | 322 | 73.079 | 5.82 | 754.004 | 1.00 | 20 00 |
| | | | ASN A | 323 | 71.579 | 4.89 | 4 126.265 | | 39.89 |
| MOTA | 2568 | | 7011 | | 72.594 | 4.06 | 7 126.895 | | 40.96 |
| ATOM | 2569 | | ASN A | 1 343 | 72.136 | | 6 128.259 | 1.00 | 43.00 |
| MOTA | 2570 | CB | ASN A | 323 | | | 6 128.202 | | 45.59 |
| ATOM | 2571 | | ASN A | 323 | 70.787 | | 0 140.404 | | 45.71 |
| | | | L ASN A | | 70.482 | 2.15 | 1 127.264 | | 40.00 |
| ATOM | 2572 | . עני | | 323 | 69.975 | 3.11 | 4 129.224 | | 48.08 |
| ATOM | 2573 | | 2 ASN A | 3 3 2 3 | | | 4 125.954 | 1.00 | 44.88 |
| MOTA | 2574 | C | ASN A | 323 | 72.828 | 4.65 | | | |
| | | | | | • | | | | |

| • | | a 201 2 222 | 72.124 | 2.739 124.955 | 1.00 46.41 |
|------|---------------|---------------|----------|----------------|------------|
| ATOM | 2575 | O ASN A 323 | | 2 062 126 268 | 1.00 45.98 |
| MOTA | 2576 | N ASN A 324 | 73.809 | 2.062 126.268 | |
| | | | 74.122 | 0.938 125.404 | 1.00 49.82 |
| MOTA | 2577 | | | 0.244 125.904 | 1.00 53.88 |
| MOTA | 2578 | CB ASN A 324 | 75.386 | 0.244 123.304 | |
| | | 4 | 75.960 | -0.711 124.888 | 1.00 60 09 |
| ATCM | 2579 | CG ASN A 324 | _ | -1.723 124.550 | 1.00 66.99 |
| MOTA | 2580 | OD1 ASN A 324 | 75.344 | -1.723 124.330 | |
| | | ND2 ASN A 324 | 77.143 | -0.386 124.378 | 1.00 58.06 |
| MOTA | 2581 | | 72.979 | -0.070 125.267 | 1.00 47.12 |
| MOTA | 2582 | C ASN A 324 | | 0.070 1251207 | 1.00 43.63 |
| | 2583 | O ASN A 324 | 72.784 | -0.644 124.197 | |
| MOTA | | | 72.220 | -0.276 126.339 | 1.00 46.39 |
| ATOM | 2584 | N LYS A 325 | | -1.221 126.318 | 1.00 46.76 |
| MOTA | 2585 | CA LYS A 325 | 71.106 | -1.221 120.310 | |
| | | | 70.428 | -1.328 127.695 | 1.00 47.65 |
| MOTA | 2586 | | | -1.837 128.858 | 1.00 54.21 |
| MOTA | 2587 | CG LYS A 325 | 71.292 | -1.657 120.636 | 1.00 56.87 |
| | 2588 | CD LYS A 325 | 72.160 | -0.750 129.526 | |
| MOTA | | | 73.329 | -0.289 128.671 | 1.00 57.45 |
| MOTA | 2589 | | | 0.816 129.307 | 1.00 58.32 |
| MOTA | 2590 | NZ LYS A 325 | 74.091 | 0.810 125.507 | 1.00 45.17 |
| | , | C LYS A 325 | 70.062 | -0.791 125.296 | |
| MOTA | 2591 | | 69.474 | -1.625 124.601 | 1.00 42.73 |
| MOTA | 2592 | O LYS A 325 | | 0.514 125.213 | 1.00 41.43 |
| MOTA | 2593 | N ALA A 326 | 69.832 | 0.514 125.215 | |
| | | CA ALA A 326 | 68.861 | 1.054 124.276 | 1.00 41.61 |
| MOTA | 2594 | | 68.562 | 2.508 124.616 | 1.00 42.80 |
| ATOM | 2595 | CB ALA A 326 | | 0.940 122.838 | 1.00 43.80 |
| MOTA | 2596 | C ALA A 326 | 69.365 | 0.940 122.030 | |
| | 2597 | O ALA A 326 | 68.595 | 0.625 121.926 | 1.00 45.17 |
| ATOM | | | 70.658 | 1.191 122.637 | 1.00 43.46 |
| ATOM | 2598 | N LYS A 327 | | 1.120 121.296 | 1.00 43.26 |
| MOTA | 25 9 9 | CA LYS A 327 | 71.235 | 1.120 121.290 | |
| | 2600 | CB LYS A 327 | 72.723 | 1.484 121.311 | 1.00 44.77 |
| MOTA | | | 73.037 | 2.892 121.800 | 1.00 50.87 |
| ATOM | 2601 | CG LYS A 327 | | 3.168 121.747 | 1.00 52.74 |
| ATOM | 2602 | CD LYS A 327 | 74.544 | 3.100 121.71 | 1.00 51.30 |
| | 2603 | CE LYS A 327 | 74.916 | 4.508 122.377 | |
| MOTA | | ^ - | 74.256 | 5.670 121.715 | 1.00 52.72 |
| MOTA | 2604 | | 71.063 | -0.274 120.728 | 1.00 41.29 |
| ATOM | 2605 | C LYS A 327 | | | 1.00 38.83 |
| ATOM | 2606 | O LYS A 327 | 70.625 | -0.437 119.592 | |
| | 2607 | N GLU A 328 | 71.403 | -1.278 121.526 | 1.00 39.95 |
| MOTA | _ | N ODO II 320 | 71.276 | -2.660 121.090 | 1.00 42.40 |
| ATOM | 2608 | CA GLU A 328 | | -3.605 122.135 | 1.00 43.05 |
| MOTA | 2609 | CB GLU A 328 | 71.875 | -3.603 122.133 | |
| | 2610 | CG GLU A 328 | 73.369 | -3.432 122.295 | |
| MOTA | | | 74.096 | -3.529 120.963 | 1.00 52.11 |
| MOTA | 2611 | | | -4.574 120.291 | 1.00 55.44 |
| MOTA | 2612 | OE1 GLU A 328 | 73.972 | 24.374 120.504 | 1.00 51.64 |
| | 2613 | OE2 GLU A 328 | 74.785 | -2.558 120.584 | |
| MOTA | | | 69.825 | -3.030 120.818 | 1.00 39.51 |
| ATOM | 2614 | | 69.536 | -3.842 119.939 | 1.00 37.35 |
| MOTA | 2615 | O GLU A 328 | | -3.042 123.502 | 1.00 36.37 |
| | 2616 | N LEU A 329 | 68.911 | -2.444 121.582 | |
| ATOM | | | 67.496 | -2.717 121.380 | 1.00 36.03 |
| atom | 2617 | | 66.646 | -1.958 122.400 | 1.00 34.66 |
| ATOM | 2618 | CB LEU A 329 | | 2 110 122 213 | 1.00 33.88 |
| ATOM | 2619 | CG LEU A 329 | 65.133 | -2.110 122.213 | 1.00 35.00 |
| | | CD1 LEU A 329 | 64.755 | -3.572 122.351 | 1.00 36.21 |
| MOTA | 2620 | CDI DEG A 329 | 64.391 | -1.268 123.240 | 1.00 34.00 |
| ATOM | 2621 | CD2 LEU A 329 | | 2 260 110 071 | 1.00 33.64 |
| ATOM | 2622 | C LEU A 329 | 67.120 | -2.268 119.971 | 1 00 33.01 |
| | | | 66.655 | -3.061 119.162 | 1.00 31.29 |
| ATOM | 2623 | | 67.333 | -0.990 119.681 | 1.00 33.78 |
| ATOM | 2624 | N LEU A 330 | | -0.461 118.366 | 1.00 36.38 |
| ATOM | 2625 | CA LEU A 330 | 67.004 | -0.401 110.300 | 1 00 20 74 |
| | | CB LEU A 330 | 67.326 | 1.033 118.294 | 1.00 30.74 |
| MOTA | 2626 | | 66.514 | 1.958 119.205 | 1.00 31.51 |
| MOTA | 2627 | CG LEU A 330 | | 3.404 118.894 | 1.00 22.11 |
| ATOM | 2628 | CD1 LEU A 330 | 66.857 | 3.404 110.034 | 1.00 29.69 |
| | | CD2 LEU A 330 | 65.028 | 1.728 118.978 | 1.00 25.05 |
| ATOM | 2629 | | | -1.201 117.246 | 1.00 36.49 |
| ATOM | 2630 | C LEU A 330 | | -1.493 116.210 | 1.00 35.61 |
| ATOM | 2631 | O LEU A 330 | 67.142 | -1.433 110.210 | 1.00 37.63 |
| | 2632 | N LYS A 331 | 69.005 | -1.503 117.455 | 1.00 37.03 |
| ATOM | | | | -2.205 116.446 | 1.00 41.32 |
| ATCM | 2633 | CA LYS A 331 | | | 1.00 44.74 |
| ATOM | 2634 | CB LYS A 331 | 71.256 | -2.272 110.074 | 1.00 44.68 |
| | 2635 | CG LYS A 331 | 71.954 | -0.919 116.869 | |
| ATOM | | | | -0.964 117.498 | 1.00 51.42 |
| ATOM | 2636 | CD LYS A 331 | | | 1.00 53./1 |
| ATOM | 2637 | CE LYS A 331 | | | |
| | 2638 | NZ LYS A 331 | . 73.928 | | |
| ATOM | | | | -3.612 116.173 | |
| atom | 2639 | | | | 1.00 42.68 |
| ATOM | 2640 | O LYS A 331 | . 05.510 | | |

| | 0641 | N SER A 332 | 68.734 | -4.270 117.200 | 1.00 41.56 |
|------------|------|---------------|----------|----------------|--------------|
| MOTA | 2641 | N SER A 332 | 68.226 | -5.629 117.039 | 1.00 46.88 |
| ATOM | 2642 | CA SER A 332 | | | 1.00 42.19 |
| ATOM | 2643 | CB SER A 332 | 68.045 | | 1.00 39.55 |
| ATOM | 2644 | OG SER A 332 | 66.959 | -5.714 119.096 | |
| | 2645 | C SER A 332 | 66.896 | -5.687 116.297 | 1.00 48.58 |
| MOTA | | | 66.393 | -6.774 116.017 | 1.00 45.78 |
| MOTA | 2646 | | 66.325 | -4.531 115.979 | 1.00 48.27 |
| MOTA | 2647 | N ILE A 333 | 65.041 | -4.503 115.292 | 1.00 51.82 |
| ATOM | 2648 | CA ILE A 333 | | -3.119 115.402 | 1.00 52.16 |
| MOTA | 2649 | CB ILE A 333 | 64.378 | | 1.00 52.64 |
| ATOM | 2650 | CG2 ILE A 333 | 63.038 | | 1.00 52.70 |
| | 2651 | CG1 ILE A 333 | 64.163 | -2.765 116.871 | 1.00 52.70 |
| MOTA | | CD1 ILE A 333 | 63.550 | -1.402 117.077 | 1.00 56.70 |
| MOTA | 2652 | | 65.112 | -4.887 113.820 | 1.00 53.43 |
| MOTA | 2653 | | 66.118 | -4.675 113.145 | 1.00 56.45 |
| MOTA | 2654 | O ILE A 333 | 64.016 | -5.461 113.344 | 1.00 55.53 |
| ATOM | 2655 | N ASP A 334 | | | 1.00 59.58 |
| MOTA | 2656 | CA ASP A 334 | 63.865 | | 1.00 62.69 |
| ATOM | 2657 | CB ASP A 334 | 62.845 | -7.040 111.918 | 1.00 66.23 |
| | 2658 | CG ASP A 334 | 61.546 | -6.712 112.664 | |
| ATOM | 2659 | OD1 ASP A 334 | 60.795 | -5.814 112.227 | 1.00 63.25 |
| ATOM. | | OD2 ASP A 334 | 61.277 | -7.354 113.704 | 1.00 63.45 |
| ATOM | 2660 | | 63.385 | -4.705 111.125 | 1.00 60.81 |
| MOTA | 2661 | C ASP A 334 | 62.239 | -4.673 110.681 | 1.00 59.47 |
| MOTA | 2662 | O ASP A 334 | | -3.736 110.889 | 1.00 60.00 |
| ATOM | 2663 | N PHE A 335 | 64.266 | -2.545 110.147 | 1.00 59.37 |
| ATOM | 2664 | CA PHE A 335 | 63.864 | | 1.00 53.38 |
| ATOM | 2665 | CB PHE A 335 | 64.247 | -1.298 110.952 | 1.00 49.13 |
| | 2666 | CG PHE A 335 | 63.895 | -0.013 110.275 | 1.00 49.13 |
| MOTA | 2667 | CD1 PHE A 335 | 62.618 | 0.189 109.770 | 1.00 44.32 |
| MOTA | | | 64.845 | 0.993 110.127 | 1.00 49.91 |
| MOTA | 2668 | | 62.288 | 1.373 109.122 | 1.00 42.74 |
| MOTA | 2669 | | 64.526 | 2.180 109.483 | 1.00 46.40 |
| MOTA | 2670 | CE2 PHE A 335 | | 2.370 108.978 | 1.00 42.77 |
| MOTA | 2671 | CZ PHE A 335 | 63.244 | -2.399 108.696 | 1.00 60.85 |
| ATOM | 2672 | C PHE A 335 | 64.334 | | 1.00 66.28 |
| ATOM | 2673 | O PHE A 335 | 63.689 | | 1.00 57.40 |
| | 2674 | N GLU A 336 | | -1:671 108.493 | |
| ATOM | 2675 | CA GLU A 336 | 66.015 | -1.411 107.174 | 1.00 58.96 |
| MOTA | 2012 | 22 | 65.782 | -2.579 106.211 | 1.00 62.66 |
| MOTA | 2676 | CB GLU A 336 | | -2.377 104.846 | 1.00 68.51 |
| · ATOM | 2677 | CG GLU A 336 | | -3.590 103.943 | 1.00 73.21 |
| MOTA | 2678 | CD GLU A 336 | | -4.678 104.333 | 1.00 73.30 |
| MOTA | 2679 | OE1 GLU A 336 | | -3.457 102.843 | 1.00 75.74 |
| ATOM | 2680 | OE2 GLU A 336 | | | 1.00 55.70 |
| MOTA | 2681 | C GLU A 336 | 65.460 | -0.124 106.576 | 1.00 55.28 |
| MOTA | 2682 | o GLU A 330 | 64.281 | -0.023 106.253 | |
| | 2683 | N GLU A 3,3° | 66.338 | 0.857 106.432 | |
| ATOM | | CA GLU A 33 | 65.986 | 2.167 105.905 | |
| MOTA | 2684 | | 67.221 | 3.065 105.983 | |
| MOTA | 2685 | | | 4.536 106.092 | 1 00 52.28 |
| ATOM | 2686 | | | 4.891 107.366 | : .00 43.72 |
| ATOM | 2687 | CD GLU A 33 | | | 2 00 42.21 |
| ATOM | 2688 | OE1 GLU A 33 | 66.705 | 00 05/ | |
| ATOM | 2589 | OE2 GLU A 33 | 65.072 | | |
| ATOM | 2690 | | 7 65.485 | | |
| | 2691 | | 7 66.087 | 1.377 103.639 | |
| ATOM | | | 64.385 | 2.745 104.151 | |
| ATOM | 2692 | | | 2.710 102.805 | 1.00 61.69 |
| MOTA | 2693 | | | | 1.00 60.86 |
| ATOM | 2694 | CB PHE A 33 | | | |
| ATOM | 2695 | CG PHE A 33 | 61.845 | | |
| ATOM | 2696 | CD1 PHE A 33 | 8 61.054 | | |
| ATOM | 2697 | | 8 61.970 | 00 06 | |
| | 2698 | | | 2.302 99.86 | |
| MOTA | | | 8 61.315 | 4.428 99.22 | |
| MOTA | 2699 | | | 3.322 98.93 | |
| ATOM | 2700 | | · | | 3 1.00 64.33 |
| ATOM | 2701 | C PHE A 33 | | 100 (1 | 6 1.00 62.45 |
| ATOM | 2702 | | | | 4 1.00 64.11 |
| ATOM | 2703 | N ASP A 33 | | | |
| ATOM | 2704 | ı CA ASPA 33 | 9 66.689 | | |
| | 2705 | CB ASP A 33 | 9 66.56 | 100 10 | |
| ATOM | 2700 | | 9 67.64 | 6.838 100.40 | Z 1.00 00.03 |
| 3 **** 150 | | | | | |

| MOTA MOTA MOTA | 2707 2708 2709 | OD1 ASP A 339 OD2 ASP A 339 C ASP A 339 | 67.796 68.346 68.088 | 4.295 101.763 | 1.00 72.20 1.00 64.15 1.00 68.73 1.00 68.17 |
|----------------------|----------------------|---|----------------------------|----------------------------------|--|
| MOTA | 2710 | O ASP A 339 | 68.511 68.796 | 4.628 102.869 3.588 100.888 | 1.00 71.90 |
| MOTA | 2711 | N ASP A 340 CA ASP A 340 | 70.151 | 3.111 101.149 | 1.00 73.59 |
| MOTA | 2712 2713 | CA ASP A 340 CB ASP A 340 | 70.778 | 2.601 99.848 | 1.00 75.47 |
| MOTA MOTA | 2714 | CG ASP A 340 | 69.953 | 1.511 99.195 | 1.00 76.03 |
| ATOM | 2715 | OD1 ASP A 340 | 69.761 | 0.449 99.823 | 1.00 76.90 1.00 80.23 |
| ATOM | 2716 | OD2 ASP A 340 | 69.492 | 1.718 98.054 4.155 101.766 | 1.00 30.22 |
| MOTA | 2717 | C ASP A 340 | . 71.069 71.618 | 3.946 102.845 | 1.00 73.08 |
| ATOM | 2718 | O ASP A 340 N GLU A 341 | 71.242 | 5.275 101.074 | 1.00 73.15 |
| MOTA | 2719 2720 | CA GLU A 341 | 72.112 | 6.341 101.557 | 1.00 74.56 |
| MOTA MOTA | 2721 | CB GLU A 341 | 72.917 | 6.924 100.390 | 1.00 77.06 1.00 82.57 |
| ATOM | 2722 | CG GLU A 341 | 73.878 | 8.034 100.792 7.571 101.794 | 1.00 85.34 |
| MOTA | 2723 | CD GLU A 341 | 74.924 75.718 | 6.669 101.450 | 1.00 86.64 |
| ATOM | 2724 | OE1 GLU A 341 OE2 GLU A 341 | 74.951 | 8.106 102.924 | 1.00 85.37 |
| ATOM | 2725 2726 | C GLU A 341 | 71.327 | 7.453 102.245 | 1.00 72.47 |
| MOTA MOTA | 2727 | O GLU A 341 | 70.822 | 8.364 101.589 | 1.00 76.75 1.00 67.86 |
| ATOM | 2728 | N VAL A 342 | 71.228 | 7.381 103.566 8.393 104.323 | 1.60 64.84 |
| MOTA | 2729 | CA VAL A 342 | 70.503 69.160 | 7.853 104.850 | 1.00 66.27 |
| MOTA | | CB VAL A 342 CG1 VAL A 342 | 68.256 | 7.494 103.701 | 1.00 67.95 |
| MOTA | 2731 2732 | CG2 VAL A 342 | 69.400 | 6.637 105.722 | 1.00 65.37 |
| ATOM ATOM | 2733 | C VAL A 342 | 71.305 | 8.871 105.520 | 1.00 61.75 1.00 64.14 |
| MOTA | 2734 | O VAL A 342 | 71.375 | 10.066 105.795 7.925 106.225 | 1.00 56.79 |
| ATOM | 2735 | N ASP A 343 | 71.912 72.692 | 8.229 107.417 | 1.00 54.53 |
| ATOM- | 2736 | CA ASP A 343 CB ASP A 343 | 73.707 | 9.340 107.158 | 1.00 56.31 |
| MOTA | 2737 2738 | CG ASP A 343 | 74.531 | 9.660 108.388 | 1.00 58.81 |
| MOTA MOTA | 2739 | OD1 ASP A 343 | 75.298 | 10.644.108.357 | 1.00 65.36 1.00 54.29 |
| MOTA | 2740 | OD2 ASP A 343 | 74.420 | 8.918 109.387 8.675 108.534 | 1.00 50.70 |
| ATOM | 2741 | C ASP A 343 | 71.765 71.442 | 9.859 108.651 | 1.00 46.00 |
| ATOM | 2742 | O ASP A 343 N ARG A 344 | 71.328 | 7.717 109.341 | 1.00 46.20 |
| MOTA MOTA | 2743 2744 | CA ARG A 344 | 70.452 | 8.004 110.463 | 1.00 41.18 1.00 39.81 |
| MOTA | 2745 | CB ARG A 344 | 69.121 | 7.268 110.299 7.711 109.098 | 1.00 35.08 |
| ATOM | 2746 | CG ARG A 344 | 68.289 68.036 | 9.211 109.121 | 1.00 28.37 |
| ATOM | 2747 | CD ARG A 344 NE ARG A 344 | 67.157 | 9.645 108.036 | 1.00 30.90 |
| MOTA | 2748 2749 | NE ARG A 344 CZ ARG A 344 | 67.013 | 10.909 107.649 | 1.00 31.05 |
| MOTA MOTA | 2750 | NH1 ARG A 344 | 67.693 | 11.874 108.258 | 1.00 30.49 1.00 31.76 |
| ATOM | 2751 | NH2 ARG A 344 | 66.201 | 11.212 106.646 7.561 111.742 | 1.00 38.46 |
| ATOM | 2752 | C ARG A 344 | 71.147 70.516 | 7.370 112.773 | 1.00 34.99 |
| ATOM | 2753 | O ARG A 344 N SER A 345 | 72.464 | 7.418 111.662 | 1.00 33.97 |
| ATOM | 2754 2755 | CA SER A 345 | 73.261 | 6.981 112.795 | |
| atom Atom | 2756 | CB SER A 345 | 74.742 | 6.972 112.404 | |
| ATOM | 2757 | OG SER A 345 | 75.163 | 8.260 111.990 7.826 114.053 | |
| MOTA | 2758 | | 73.054 73.100 | 7.314 115.167 | 1.00 24.35 |
| ATOM | 2759 2760 | | 72.819 | 9.119 113.877 | 1.00 33.10 |
| MOTA MOTA | 2761 | | 72.614 | 10.003 115.015 | 1.00 34.50 |
| MOTA | 2762 | CB TYR A 346 | 72.397 | 11.437 114.522 | 1.00 35.16 |
| ATOM | 2763 | CG TYR A 346 | 71.168 | 11.615 113.659 11.814 114.227 | |
| MOTA | 2764 | | 69.909 68.767 | 11.940 113.424 | 1.00 40.23 |
| ATOM | 2765 | | 71.260 | 11.544 112.270 | 1.00 39.04 |
| ATOM | 2766 2767 | | 70.131 | 11.667 111.463 | |
| atom atom | 2768 | CZ TYR A 346 | 68.890 | 11.864 112.041 | |
| ATOM | 2769 | OH TYR A 346 | 67.776 | 11.982 111.234 9.560 115.874 | 1.00 37.72 |
| MOTA | 2770 | | 71.432 71.396 | 9.829 117.074 | 1.00 35.48 |
| ATCM | 2771 | | 70.472 | 8.869 115.269 | |
| ATCM | 2772 | | • | | |

| | | | | * -6 | , | | | |
|--|--|--|--|------|--|---|--------------------|--|
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 2773 2774 2775 2776 2777 2778 2779 2780 2781 2782 2783 2784 2785 2786 2787 2788 | CB M CG M SD M CE M C O M N L CA L CB L CG I CD1 I CD2 I C O I N C | ET A 347 IET A 348 IEU A 348 | - | 69.295 68.226 67.853 66.471 67.058 69.632 68.890 70.747 71.137 71.841 71.066 72.010 69.906 72.075 72.583 72.295 | 7.868 8.809 8.194 6.647 7.363 7.187 6.663 5.641 4.476 3.655 2.660 2.935 6.232 5.513 7.541 | 115.052 | 1.00 36.97 1.00 33.45 1.00 28.09 1.00 32.14 1.00 39.25 1.00 34.67 1.00 36.42 1.00 34.57 1.00 34.16 1.00 36.58 1.00 36.58 1.00 42.34 1.00 37.75 1.00 38.31 1.00 42.86 |
| MOTA | 2789 | CA (| GLU A 349 | | 73.192 | 8.231 | 118.948 | 1.00 47.04 |
| ATOM | 2790 | | GLU A 349 | | 74.150 | 9.136 | 117.867 | 1.00 53.27 |
| ATOM | 2791 | | GLU A 349 | | 74.942 | 8.420 | 118.410 | 1.00 58.36 |
| ATOM | 2792 | CD (| GLU A 349 | | 75.828 | 7.323 | 119.279 | 1.00 59.59 |
| ATOM | 2793 | OE1 (| GLU A 349 | | 76.681 | 6 166 | 117.963 | 1.00 59.17 |
| ATOM | 2794 | OE2 | GLU A 349 | | 75.669 | 0.100 | 120.752 | 1.00 41.72 |
| MOTA | 2795 | C | GLU A 349 | | 72.458 72.564 | 8 852 | 121.959 | 1.00 42.27 |
| MOTA | 2796 | 0 (| GLU A 349 | | 71.716 | 10.067 | 120.261 | 1.00 37.05 |
| MOTA | 2797 | N | THR A 350 THR A 350 | | 70.992 | 10.976 | 121.135 | 1.00 40.78 |
| MOTA | 2798 | CA | THR A 350 | | 71.468 | 12.418 | 120.900 | 1.00 41.69 |
| MOTA | 2799 2800 | CB OG1 | THR A 350 | | 71.359 | 12.733 | 119.508 | 1.00 43.25 |
| MOTA MOTA | 2801 | | THR A 350 | | 72.918 | 12.575 | 121.325 | 1.00 44.11 |
| ATOM | 2802 | | THR A 350 | | 69.474 | 10.911 | 120.968 | 1.00 41.47 1.00 39.72 |
| ATOM | 2803 | 0 | THR A 350 | | 68.968 | 10.608 | 119.884 122.054 | 1.00 38.68 |
| ATOM | 2804 | N | LEU A 351 | | 68.760 | 11.199 | 122.056 | 1.00 35.91 |
| MOTA | 2805 | | LEU A 351 | | 67.299 66.763 | 11.103 | 123.487 | 1.00 35.94 |
| ATOM | 2806 | | LEU A 351 | | 66.752 | 9.890 | 124.251 | 1.00 37.67 |
| MOTA | 2807 | CG | LEU A 351 | | 66.290 | 10.118 | 125.677 | 1.00 40.11 |
| MOTA | 2808 | CD1 | LEU A 351 LEU A 351 | | 65.813 | 8.920 | 123.544 | 1.00 39.29 |
| MOTA | 2809 2810 | CD2 | LEU A 351 | | 66.679 | 12.342 | 121.294 | 1.00 37.76 |
| ATOM | 2811 | 0 | LEU A 351 | | 65.747 | 12.149 | 120.512 | 1.00 34.86 |
| MOTA MOTA | 2812 | N | LYS A 352 | | 67.192 | 13.544 | 121.525 | 1.00 34.79 1.00 38.73 |
| ATOM | 2813 | CA | LYS A 352 | | 66.651 | 14.724 | 120.870 | 1.00 36.48 |
| ATOM | 2814 | CB | LYS A 352 | | 66.676 | 15.911 | 121.835 123.179 | 1.00 42.08 |
| ATOM | 2815 | CG | LYS A 352 | | 66.062 | 15.300 | 124.196 | 1.00 43.22 |
| ATOM | 2816 | CD | LYS A 352 | | 66.202 | 17 901 | 123.845 | 1.00 49.81 |
| ATOM | 2817 | CE | LYS A 352 | | 65.349 65.342 | 18.880 | 124.972 | 1.00 52.70 |
| MOTA | 2818 | | LYS A 352 LYS A 352 | | 67.425 | 15.063 | 119.610 | 1.00 38.// |
| MOTA | 2819 2820 | С 0 | LYS A 352 | | 68.654 | 15.098 | 119.601 | 1.00 36.21 |
| MOTA | 2821 | | ASP A 353 | | 66.697 | 15.293 | 118.530 | 1.00 37.69 |
| MOTA | 2822 | | ASP A 353 | | 6 7 .337 | 15.647 | 117.286 | 1.00 39.89 |
| ATOM ATOM | 2823 | | ASP A 353 | | 66.532 | 15.075 | 116.110 | 1.00 43.53 1.00 47.99 |
| ATOM | 2824 | | ASP A 353 | | 65.058 | 15.368 | 116.211 | 1.00 47.33 |
| ATOM | 2825 | OD1 | ASP A 353 | | 64.253 | 14.62 | 115.593 116.898 | 1.00 52.94 |
| ATOM | 2826 | OD2 | ASP A 353 | | 64.706 | 10.304 | 117.247 | 1.00 39.20 |
| ATOM | 2827 | C | ASP A 353 | | 67.457 | 17.10 | 118.092 | 1.00 35.66 |
| MOTA | 2828 | | ASP A 353 | | 66.890 68.244 | 17.60 | 5 116.302 | |
| MOTA | 2829 | | PRO A 354 | | 69.047 | 17.00 | 5 115.279 | 1.00 40.05 |
| MOTA | 2830 | | PRO A 354 | | 68.426 | 19.14 | 5 116.179 | 1.00 38.41 |
| MOTA | 2831 | | PRO A 354 PRO A 354 | | 69.534 | 19.25 | 0 115.140 | 1.00 36.24 |
| MOTA | 2832 | | PRO A 354 | | 69.190 | 18.09 | 5 114.225 | 1.00 39.41 |
| ATOM | 2833 | | PRO A 354 | | 67.144 | 19.78 | 0 115.689 | 1.00 37.28 |
| MOTA | 2834 2835 | | PRO A 354 | | 66.299 | 19.10 | 6 115.094 | 1.00 31.8/ |
| MOTA | 2836 | | TRP A 355 | | 66.993 | 21.07 | 4 115.934 | |
| MOTA | 2837 | | TRP A 355 | | 65.804 | | 7 115.472 | |
| ATOM | 2838 | | TRP A 355 | | 65.714 | 23.15 | 7 116.080 | 1.00 42.03 |
| MOTA | 2000 | | | | | | | |

| | 2020 | CG TRP | A 355 | 64 | . 333 | 23.471 | 116.569 | 1.00 5 | |
|------|--------------|---------|----------------|-----|--------|---------|-----------|--------|-------|
| MOTA | 2839 | | A 355 | | 439 | | 116.047 | 1.00 5 | |
| MOTA | 2840 | | A 355 | | . 234 | 24.368 | 116.783 | 1.00 5 | |
| MOTA | 2841 | | A 355 | | .538 | 25.422 | 115.028 | 1.00 5 | |
| MOTA | 2842 | | | | . 655 | 22.836 | 117.575 | 1.00 5 | 1.80 |
| MOTA | 2843 | | A 355 | | . 393 | | 117.708 | 1.00 5 | 1.38 |
| MOTA | 2844 | | A 355 | | .134 | | 116.532 | 1.00 5 | 1.28 |
| ATOM | 2845 | | A 355 | | .444 | | 114.779 | 1.00 5 | |
| MOTA | 2846 | | A 355 | | . 257 | 26.126 | 115.531 | 1.00 5 | 0.50 |
| MOTA | 2847 | | A 355 | | .935 | 21.836 | 113.954 | 1.00 3 | |
| MOTA | 2848 | | A 355 | 63 | .041 | 21.929 | 113.422 | 1.00 3 | |
| MOTA | 2849 | | A 355 | | .809 | 21.764 | 113.259 | 1.00 3 | |
| MOTA | 2850 | N ARG | A 356 | | .797 | 21.820 | 111.802 | 1.00 3 | |
| MOTA | 2851 | | A 356 | | . 317 | 20.469 | 111.252 | 1.00 | 33.36 |
| MOTA | 2852 | CB ARG | A 356 | | .310 | 19.340 | 111.564 | 1.00 | 34.50 |
| ATOM | 2853 | | A 356 | 51 | .729 | 17.927 | 111.468 | 1.00 2 | |
| MOTA | 2854 | CD ARG | A 356 | 65 | .745 | 16.956 | 111.870 | 1.00 | 24.79 |
| MOTA | 2855 | _ | A 356 | | .499 | 15.703 | 112.236 | 1.00 | 27.56 |
| MOTA | 2856 | CZ ARG | A 356 | | .253 | 15.237 | 112.259 | 1.00 | 19.09 |
| MOTA | 2857 | NH1 ARG | A 356 | 66 | .502 | 14.918 | 112.604 | 1.00 | 21.34 |
| MOTA | 2858 | | A 356 | 63 | .874 | 22.955 | 111.390 | 1.00 | 33.74 |
| ATOM | 2859 | | A 356 | | .746 | 22.732 | 110.950 | 1.00 | 34.68 |
| MOTA | 2860 | | A 356 | | .361 | 24.181 | 111.550 | 1.00 | 35.60 |
| MOTA | 2861 | | A 357 | | .556 | 25.345 | 111.220 | 1.00 | 35.43 |
| MOTA | 2862 | | A 357 | 6.3 | .719 | 25.932 | 109.830 | | 38.08 |
| MOTA | 2863 | | A 357 | | .112 | 25.250 | | | 37.29 |
| MOTA | 2864 | O GLY | A 357 A 358 | | .406 | 27.218 | | 1.00 | 39.67 |
| ATOM | 2865 | | A 358 | | 3.493 | 27.925 | | 1.00 | 36.36 |
| MOTA | 2866 | | | | 2.398 | 28.966 | 108.499 | | 39.45 |
| MOTA | 2867 | C GLY | | 61 | .763 | 29.131 | 109.539 | | 37.58 |
| MOTA | 2868 | | A 350 | | 2.163 | 29.662 | 107.391 | | 40.89 |
| MOTA | 2869 | | | | 1.121 | 30.682 | | | 41.37 |
| MOTA | 2870 | CA GLU | A 359 | | 1.310 | 31.627 | | | 44.64 |
| MOTA | 2871 | | J A 359 | | 0.956 | 30.977 | 104.848 | 1.00 | 52.13 |
| MOTA | 2872 | CG GLU | J A 359 | | 0.833 | 31.973 | | | 59.14 |
| MOTA | 2873 | | J A 359 | | 0.448 | 31.551 | | | 60.47 |
| MOTA | 2874 | | J A 359 | | 1.119 | 33.173 | 103.923 | | 57.77 |
| ATOM | 2875 | | J A 359 | | 9.770 | 30.006 | 107.200 | 1.00 | 38.02 |
| MOTA | 2876 | | J A 359 | | 9.689 | 28.828 | 106.850 | 1.00 | 35.29 |
| ATCM | 2877 | | A 360 | | 8.708 | 30.762 | 107.441 | 1.00 | 36.81 |
| ATOM | 2878 | | L A 360 | | 7.363 | 30.237 | 107.291 | | 35.97 |
| MOTA | 2879 2880 | | L A 360 | | 6.401 | 30.789 | 108.368 | | 34.90 |
| ATOM | | | L A 360 | | 4.999 | 30.251 | 108.133 | | 36.53 |
| MOTA | 2881 2882 | | L A 360 | | 6.888 | 30.393 | 3 109.755 | | 37.06 |
| ATOM | 2883 | | L A 360 | | 6.886 | 30.690 | 105.928 | 1.00 | 36.74 |
| ATOM | 2884 | | L A 360 | | 6.661 | 31.883 | 1 105.712 | 1.00 | 34.90 |
| ATOM | 2885 | | G A 361 | | 6.753 | 29.74 | 1 105.004 | 1.00 | 35.48 |
| MOTA | 2886 | CA AR | G A 361 | | 6.301 | 30.04 | 9 103.652 | 1.00 | 38.21 |
| ATOM | 2887 | CB AR | G A 361 | 5 | 6.152 | 28.77 | 6 102.815 | 1.00 | 39.76 |
| ATOM | 2888 | CG AR | G A 361 | 5 | 7.416 | | 2 102.098 | | 39.93 |
| ATOM | 2889 | | G A 361 | | 7.225 | 26.96 | 3 101.486 | | 38.68 |
| ATOM | 2890 | | G A 361 | | 7.112 | 25.94 | 0 102.525 | | 39.72 |
| ATCM | 2891 | | G A 361 | 5 | 6.952 | 24.64 | 3 102.286 | | 38.79 |
| ATOM | 2891 | | G A 361 | 5 | 6.881 | 24.20 | 0 101.036 | | 32.40 |
| MOTA | 2892 | NH2 AR | G A 361 | | 6.899 | 23.78 | 5 103.297 | | 36.58 |
| MOTA | 2893 2894 | | G A 361 | | 4.996 | 30.80 | 7 103.603 | | 38.98 |
| ATOM | 2895 | | G A 361 | | 4.120 | 30.63 | 6 104.452 | | 39.07 |
| ATOM | 2895 | | S A 362 | 5 | 4.880 | 31.63 | 4 102.573 | | 39.95 |
| ATCM | 2897 2897 | | S A 362 | 5 | 3.709 | 32.45 | 9 102.339 | | 42.73 |
| ATOM | | | S A 362 | | 3.931 | . 33.30 | 1 101.078 | 1.00 | 44.92 |
| ATOM | 2898 | | S A 362 | 5 | 4.995 | 34.39 | | | 55.45 |
| ATOM | 2899 | | S A 362 | - | 6.351 | 33.84 | 2 101.671 | | 58.28 |
| ATCM | | | S A 362 | 5 | 6.907 | 7 32.80 | 9 100.697 | | 57.34 |
| ATOM | | | S A 362 | 9 | 58.224 | 32.28 | 3 101.151 | | 58.75 |
| ATOM | | | S A 362 | | 52.434 | 1 31.63 | 4 102.200 | | 40.51 |
| ATOM | 2903 | | S A 362 | | 31.391 | | 6 102.748 | 1.00 | 36.10 |
| ATOM | 2904 | | | | | | | | |

| | | | | 4 | 9 | _ | | | |
|--|--|---|--|---|--|--|--|--|--|
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 2905 2906 2907 2908 2909 2910 2911 2912 2913 2914 2915 2916 2917 | CA GLU CB GLU CG GLU CD GLU OE1 GLU OE2 GLU C GLU N VAI CA VAI CB VAI CG1 VAI | J A 363 J A 363 J A 363 J A 363 J A 363 J A 363 J A 364 L A 364 L A 364 L A 364 | | 52.506 51.313 51.587 52.729 52.995 52.080 54.116 50.788 49.582 51.691 51.274 52.484 52.018 53.198 | 30.527 29.705 28.530 27.616 26.547 25.737 26.526 29.209 29.113 28.910 28.455 28.048 27.676 26.867 | 101.295 100.347 100.739 99.683 99.409 99.125 102.636 102.834 103.564 104.886 105.749 107.160 105.109 | 1.00 3 1.00 4 1.00 4 1.00 5 1.00 4 1.00 3 1.00 3 1.00 3 1.00 3 | 0.96 3.62 7.01 1.65 5.63 8.44 7.74 4.79 3.64 2.39 3.99 |
| ATOM ATOM | 2918 2919 | C VA | L A 364 | | 50.506 | 29.574 | 105.589 | 1.00 3 | 4.33 |
| MOTA | 2920 | O VA | L A 364 | | 49.454 | 29.336 30.797 | 106.188 105.499 | 1.00 2 | 88.12 |
| MOTA | 2921 | N LY | S A 365 S A 365 | | 51.027 50.381 | 31.952 | 106.119 | 1.00 3 | 36.77 |
| MOTA MOTA | 2922 2923 | CB LY | S A 365 | | 51.255 | 33.204 | 105.969 | 1.00 3 | 37.98 |
| ATOM | 2924 | CG LY | S A 365 | | 52.629 53.449 | 33.084 | 106.610 106.429 | 1.00 | 35.50 |
| MOTA | 2925 | | S A 365 S A 365 | | 54.837 | 34.190 | 107.032 | 1.00 4 | 40.35 |
| MOTA MOTA | 2926 2927 | CE LY | S A 365 | | 55.674 | 35.407 | 106.877 | 1.00 | 43.74 |
| ATOM | 2928 | C LY | S A 365 | | 49.025 | 32.191 | 105.468 106.148 | 1.00 | 33.53 |
| MOTA | 2929 | | S A 365 P A 366 | | 48.038 48.968 | 32.409 | 104.147 | 1.00 | 37.05 |
| ATOM | 2930 2931 | | P A 366 | | 47.708 | 32.278 | 103.449 | 1.00 | 37.72 |
| MOTA MOTA | 2932 | CB AS | P A 366 | | 47.906 | 32.237 | 101.929 | 1.00 | 40.57 43.98 |
| ATOM | 2933 | CG AS | P A 366 | | 48.833 49.078 | 33.334 34.304 | | 1.00 | 38.51 |
| ATOM | 2934 2935 | | P A 366 P A 366 | | 49.297 | 33.235 | 100.269 | 1.00 | |
| MOTA MOTA | 2935 | C AS | P A 366 | | 46.670 | 31.238 | 103.862 | 1.00 1.00 | |
| MOTA | 2937 | O AS | P A 366 | | 45.497 | 31.562 | 104.029 | 1.00 | |
| MOTA | 2938 | | IR A 367 IR A 367 | | 47.096 46.167 | 28.935 | 104.432 | 1.00 | 36.80 |
| MOTA | 2939 2940 | | IR A 367 | | 46.868 | 27.560 | 104.527 | 1.00 | 33.84 |
| MOTA MOTA | 2941 | OG1 TH | IR A 367 | | 47.332 | 27.167 | 7 103.232 9 105.046 | 1.00 | 34.92 35.11 |
| ATOM | 2942 | | IR A 367 | | 45.904 45.532 | 29.257 | | 1.00 | 36.58 |
| MOTA | 2943 | C TH | ir A 367 ir A 367 | | 44.307 | 29.202 | 2 105.931 | | 30.18 |
| MOTA MOTA | 2944 2945 | N LI | EU A 368 | | 46.363 | 29.582 | | 1.00 | 35.32 35.46 |
| ATOM | 2946 | CA LI | EU A 368 | | 45.850 | 29.926 30.169 | | | 34.03 |
| MOTA | 2947 | | EU A 368 EU A 368 | | 46.997 47.545 | | | 1.00 | 39.04 |
| MOTA MOTA | 2948 2949 | CG LI | EU A 368 | | 46.449 | 28.35 | 8 110.688 | | 37.35 |
| MOTA | 2950 | CD2 L | EU A 368 | | 48.014 | | 1 108.797 6 107.994 | | 39.52 38.12 |
| ATOM | 2951 | C LI | EU A 368 | | 44.957 43.968 | | 7 108.719 | | 31.70 |
| MOTA | 2952 | 0 L | EU A 368 LU A 369 | | 45.307 | 32.06 | 3 107.086 | 1.00 | 40.45 |
| MOTA MOTA | 2953 2954 | N G | LU A 369 | | 44.509 | 33.26 | 1 106.866 | 1.00 | 45.36 47.38 |
| ATOM | 2955 | CB G | LU A 369 | | 45.128 | | | 1.00 | 53.81 |
| MOTA | 2956 | CG G | LU A 369 | | 46.020 45.227 | | 6 106.996 | 1.00 | 59.97 |
| MOTA | 2957 | CD G | LU A 369 LU A 369 | | 45.846 | | 2 107.526 | 1.00 | 60.65 |
| ATOM | 2958 2959 | | LU A 369 | | 43.980 | 36.21 | 1 107.016 | | 63.69 43.23 |
| MOTA MOTA | 2960 | C G | LU A 369 | | 43.100 | | | | 44.62 |
| ATOM | 2961 | | LU A 369 | | 42.130 42.983 | | | 1.00 | 40.34 |
| MOTA | 2962 2963 | _ | YS A 370 YS A 370 | | 41.666 | 31.63 | 1 104.977 | 1.00 | 43.36 |
| MOTA MOTA | 2963 | CB L | YS A 370 | | 41.738 | 30.77 | | | 44.79 48.93 |
| ATOM | 2965 | CG L | YS A 370 | | 42.032 | 31.54 31.51 | | 1.00 | 51.41 |
| ATOM | 2966 | CD L | YS A 370 YS A 370 | | 43.503 43.923 | 30.11 | | 1.00 | 51.14 |
| ATOM | 2967 2968 | _ | YS A 370 | | 45.339 | 30.06 | 2 101.091 | 1.00 | 50.34 |
| MOTA · | 2969 | CI | ys A 370 | | 40.959 | | 18 106.069 | | 43.09 |
| ATOM | 2970 | | YS A 370 | | 39.745 | 30.97 | 77 106.248 | | |
| | | | | | | | | | |

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|--------------|--------------|---|--------------|---------|--------------------|--------------------------------|------|
| ATOM | 2971 2972 | N ALA A 371 CA ALA A 371 | 41.7 41.1 | 20 29.2 | 38 107.8 | 61 1.00 43.57 | 7 |
| MOTA | 2972 | CB ALA A 371 | 42.1 | 93 28.4 | 40 108.5 | | |
| MOTA | 2974 | C ALA A 371 | 40.3 | 65 30.1 | _ | 37 1.00 46.10 | |
| MOTA MOTA | 2975 | O ALA-A 371 | 39.2 | | | 10 1.00 46.07 | |
| ATOM | 2976 | N LYS à 372 | 40.9 | 81 31.2 | 39 109.2 | | |
| ATOM | 297.7 | CA LYS A 372 | 40.3 | | | | |
| MOTA | 2978 | C LYS A 372 | 39.0 | | | | |
| ATOM | 2979 | O LYS A 372 | 38.2 | | | - | |
| ATOM | 2980 | CB LYS A 372 | 41.3 | | _ | | |
| MOTA | 2981 | CG LYS A 372 | 42.8 | | | | |
| MOTA | 2982 | CD LYS A 372 | 45.2 | | | 49 1.00 20.0 | |
| MOTA | 2983 | CE LYS A 372 NZ LYS A 372 | 46.3 | | _ | 81 1.00 20.0 | |
| MOTA | 2984 | NZ LYS A 372 N ALA A 373 | 38.7 | | 476 108.3 | | |
| ATOM | 2985 2986 | CA ALA A 373 | 37.4 | 192 32. | | | |
| MOTA MOTA | 2987 | CB ALA A 373 | 37.7 | | 632 106.4 | | |
| ATOM | 2988 | C ALA A 373 | 36.9 | | 773 107.5 | | |
| MOTA | 2989 | O ALA A 373 | 35.4 | | | | |
| MOTA | 2990 | OXT ALA A 373 | 36. | 370 30. | 431 56.8 | | 7 |
| MOTA | 3014 | CB ALA B 2 | 54.8 53.9 | | | | |
| MOTA | 3015 | C ALA B 2 | 54.: | | 720 57. | | |
| MOTA | 3016 | O ALA B 2 N ALA B 2 | 54. | | 672 54.5 | 557 1.00 58.2 | 2 |
| MOTA | 3017 | | 53. | 914 -3. | 584 56.0 | 008 1.00 58.4 | 7 |
| ATOM | 3018 | CA ALA B 2 N LYS B 3 | 52. | | 376 56.3 | | 9 |
| ATOM | 3019 3020 | CA LYS 3 | 52. | | 022 56. | | |
| MOTA MOTA | 3021 | CB LYS B 3 | 51. | | 700 55. | | |
| ATOM | 3022 | CG LYS B 3 | 51. | | 785 54. | | |
| ATOM | 3023 | CD LYS 3 | 50. | | 681 53. 783 52. | | |
| ATOM | 3024 | CE LYS B 3 | 50. | | 783 52. 323 51. | | |
| MOTA | 3025 | NZ LYS B 3 | | | 238 58. | | |
| MOTA | 3026 | C LYS B 3 O LYS B 3 | | | | 830- 1.00 41.6 | 53 |
| MOTA | 3027 | | | | 385 58. | 467 1.00 41.4 | 16 |
| MOTA | 3028 3029 | N VAL B 4 CA VAL B 4 | - | 483 1. | .751 59. | | 35 |
| MOTA MOTA | 3030 | CB VAL B -4 | 54. | | .288 60. | | 22 |
| ATOM | 3031 | CG1 VAL B 4 | | • | .541 61. | | 36 |
| ATOM | 3032 | CG2 VAL B 4 | | | | 652 1.00 38.5 230 1.00 38.5 | |
| MOTA | 3033 | C VAL B 4 | | | | 691 1.00 42. | во |
| MOTA | 3034 | O VAL B 4 | | | | 157 1.00 34. | 90 |
| MOTA | 3035 | N LYS B 5 | | | 396 61. | 558 1.00 31. | 22 |
| ATOM | 3036 | CA LYS B 5 | | | .796 61. | 215 1.00 33. | |
| ATOM | 3037 | CG LYS B 5 | | 841 2 | .623 59. | 726 1.00 36. | 60 |
| MOTA | 3038 3039 | | | 667 3 | _ | 032 1.00 41. | 48 |
| MOTA MOTA | 3040 | CE LYS B 5 | | _ | · | 577 1.00 43. 781 1.00 42. | 52 |
| MOTA | 3041 | NZ LYS 3 5 | | | | 781 1.00 42. 038 1.00 32. | |
| ATOM | 3042 | C LYS B 5 | | | | 878 1.00 25. | 78 |
| MOTA | 3043 | O LYS B 5 | | | | 343 1.00 27. | 07 |
| ATOM | 3044 | | | | | 712 1.00 31. | 09 |
| MOTA | 3045 | | | | .696 64 | .896 1.00 30. | 13 |
| ATOM | 3046 | | | | .340 66 | .285 1.00 28. | 09 |
| ATOM | 3047 | | | .333 7 | .827 66 | .728 1.00 38. | 87 |
| ATOM | 3048 3049 | · • • • • • • • • • • • • • • • • • • • | | | 3.338 67 | .282 1.00 24. | 87 |
| ATOM | 3050 | | 48 | .324 5 | | .924 1.00 29. | 36 |
| MOTA MOTA | 3050 | O LEU B 6 | 47 | | | .149 1.00 33. .960 1.00 28. | 02 |
| MOTA | 3052 | N ILE B 7 | 47 | | | | 83 |
| ATOM | 3053 | 3 CA ILE 3 | | | | .250 1.00 23. .670 1.00 25. | 11 |
| ATOM | 3054 | I CB ILE B 7 | | | | .127 1.00 23 | . 59 |
| ATOM | 3055 | G CG2 ILE B 7 | | | | 477 1.00 31 | . 00 |
| ATOM | 3056 | | | | | .906 1.00 38 | . 60 |
| ATOM | 3057 | , | _ | | 5.130 67 | .363 1.00 26 | . 49 |
| ATOM | 3058 | | 46 | | | .430 1.00 26 | . 68 |
| MOTA | 3059 | 9 O ILE B | 30 | - ' | | | |

| | | | CT V D | 8 | | 45.372 | 7.151 | 67.106 | 1.00 29.51 |
|--------------|--------------|------|----------------|----------|---|------------------|------------------|------------------|--------------------------|
| ATOM | 3060 | - | GLY B | 8 | | 45.151 | 8.170 | 68.117 | 1.00 30.28 |
| ATOM | 3061 | CA | GLY B | | | 44.217 | 9.273 | 67.667 | 1.00 28.79 |
| ATOM | 3062 | С | GLY B | 8 | | 43.629 | 9.207 | 66.590 | 1.00 19.70 |
| ATOM | 3063 | 0 | GLY B | 8 | | 44.088 | 10.291 | 68.509 | 1.00 26.46 |
| ATOM | 3064 | N | THR B | 9 | | 43.234 | 11.438 | 68.238 | 1.00 29.37 |
| ATOM- | 3065 | CA | THR B | 9 | | 41.748 | 11.064 | 68.311 | 1.00 32.64 |
| atom | 3066 | CB | THR B | 9 | | 40.959 | 12.253 | 68.218 | 1.00 30.35 |
| MOTA | 3067 | OG1 | THR B | 9 | | 41.431 | 10.383 | 69.637 | 1.00 33.42 |
| MOTA | 3068 | | THR B | 9 | | 41.431 | 12.496 | 69.302 | 1.00 33.42 |
| ATOM | 3069 | С | THR B | 9 | | | 12.173 | 70.416 | 1.00 30.46 |
| ATOM | 3070 | 0 | THR B | 9 | | 43.884 | 13.754 | 68.961 | 1.00 32.05 |
| ATOM | 3071 | N | LEU B. | 10 | _ | 43.228 43.396 | 14.840 | 69.914 | 1.00 34.75 |
| ATOM | 3072 | CA | LEU B | 10 | | 43.390 | 16.189 | 69.190 | 1.00 38.02 |
| MOTA | 3073 | CB | LEU B | 10 | | 44.605 | 16.578 | 68.355 | 1.00 40.82 |
| MOTA | 3074 | CG | LEU B | 10 | | 44.961 | 15.472 | 67.394 | 1.00 43.62 |
| ATOM | 3075 | CD1 | LEU B | 10 | | 44.314 | 17.869 | 67.605 | 1.00 34.99 |
| ATOM | 3076 | | LEU B | 10 | | 42.272 | 14.809 | 70.945 | 1.00 34.25 |
| ATOM | 3077 | C | LEU B | 10 | | 42.415 | 15.348 | 72.042 | 1.00 33.13 |
| ATOM | 3078 | 0 | LEU B | 10 | | 41.158 | 14.169 | 70.595 | 1.00 30.61 |
| MOTA | 3079 | N | ASP B | 11 | | 40.011 | 14.098 | 71.501 | 1.00 33.08 |
| MOTA | 3080 | CA | ASP B | 11 | | 38.928 | 13.167 | 70.945 | 1.00 37.57 |
| MOTA | 3081 | CB | ASP B | 11 | | 38.372 | 13.643 | 69.621 | 1.00 43.14 |
| ATOM | 3082 | CG | ASP B | 11 11 | | 38.013 | 14.834 | 69.525 | 1.00 42.22 |
| MOTA | 3083 | | ASP B | 11 | | 38.281 | 12.825 | 68.681 | 1.00 45.58 |
| MOTA | 3084 | | ASP B | 11 | | 40.358 | 13.654 | 72.919 | 1.00 32.19 |
| MOTA | 3085 | C | ASP B | 11 | | 39.688 | 14.053 | 73.875 | 1.00 23.44 |
| MOTA | 3086 | 0 | ASP B | 12 | | 41.386 | 12.822 | 73.066 | 1.00 28.02 |
| MOTA | 3087 | N | TYR B | 12 | | 41.770 | 12.373 | 74.402 | 1.00 32.00 |
| ATOM | 3088 | CA | TYR B | 12 | | 43.011 | 11.476 | 74.363 | 1.00 28.67 |
| ATOM | 3089 | CB | TYR B TYR B | 12 | | 42.821 | 10.108 | 73.737 | 1.00 25.33 |
| MOTA | 3090 | CG | | 12 | | 43.338 | 9.823 | 72.475 | 1.00 23.74 |
| MOTA | 3091 | CD1 | | 12 | | 43.235 | 8.546 | 71.924 | 1.00 22.85 |
| ATOM | 3092 | CD2 | | 12 | | 42.183 | 9.077 | 74.436 | 1.00 21.93 |
| ATOM | 3093 | CE2 | | 12 | | 42.074 | 7.793 | 73.889 | 1.00 21.99 |
| MOTA | 3094 3095 | CZ | TYR B | 12 | | 42.605 | 7.538 | 72.640 | 1.00 22.99 |
| MOTA | 3095 | OH | TYR B | 12 | | 42.532 | 6.273 | 72.109 | 1.00 18.79 |
| ATOM | 3097 | C | TYR B | 12 | | 42.054 | 13.567 | 75.319 | 1.00 32.74 |
| MOTA | 3098 | ō | TYR B | 12 | | 41.986 | 13.450 | 76.542 | 1.00 23.85 |
| MOTA | 3099 | N | GLY B | 13 | | 42.374 | 14.710 | 74.720 | 1.00 26.96 1.00 34.92 |
| MOTA MOTA | 3100 | CA | GLY B | 13 | | 42.658 | 15.900 | 75.501 | 1.00 34.92 |
| ATOM | 3101 | c | GLY B | 13 | | 41.452 | 16.396 | 76.277 | 1.00 34.10 |
| ATOM | 3102 | Ö | GLY B | 13 | | 41.580 | 17.228 | 77.176 | 1.00 37.23 |
| ATOM | 3103 | N | LYS B | 14 | | 40.279 | 15.875 | 75.929 | 1.00 41.77 |
| ATOM | 3104 | CA | LYS B | 14 | | 39.031 | 16.247 | 76.584 75.537 | 1.00 45.82 |
| ATOM | 3105 | CB | LYS B | 14 | | 37.925 | 16.406 | 74.579 | 1.00 51.38 |
| ATOM | 3106 | | LYS B | 14 | | 38.110 | 17.585 | 75.241 | 1.00 57.78 |
| ATOM | 3107 | | LYS B | 14 | | 37.805 | 18.939 | | 1.00 58.82 |
| ATOM | 3108 | | LYS B | 14 | | 38.752 | 19.285 20.568 | | 1.00 55.06 |
| ATOM | 3109 | NZ | | 14 | | 38.387 | 15.226 | | |
| ATOM | 3110 | C | LYS B | 14 | | 38.591 | 15.385 | | 1.00 35.54 |
| MOTA | 3111 | . 0 | LYS B | | | 37.546 | 14.186 | | |
| ATOM | 3112 | N | TYR B | | | 39.395 | | | |
| MOTA | 3113 | CA | | | | 39.070 | | | |
| MOTA | 3114 | CB | | | | 38.863 | | | 1.00 42.02 |
| ATCM | 3115 | CG | | | | 37.850 | | | 1.00 41.06 |
| ATOM | 3116 | | | | | 38.064 37.138 | | | 1.00 42.76 |
| ATOM | 3117 | CE | | _ | | | | | 1.00 42.99 |
| ATOM | 3118 | G CE | | | | 36.678 35.748 | | | 1.00 43.30 |
| ATOM | 3119 | | | 15 | | 35.740 | | • | 1.00 45.49 |
| ATOM | 3120 | | | | | 35.964 | | _ | 1.00 45.69 |
| ATOM | 3123 | ı oh | | | | 40.151 | | | 1.00 43.48 |
| ATOM | 312 | | TYR E | | | 40.131 | | | 1.00 41.20 |
| ATOM | 312 | | TYR I | | | 40.513 | 14.05 | | 1.00 43.01 |
| ATCM | 312 | | ARG I | | | 41.686 | 14.01 | | 40 70 |
| 3.0014 | | s ca | ARG I | 3 16 | | 41.000 | | | |

| | | | | | 8 | | _ | | |
|--------------|--------------|----------|---------|----------|----|-----------------|------------------|------------------|--------------------------|
| > mo>/ | 3126 | СВ | ARG B | 16 | 42 | . 250 | 15.410 | 81.663 | 1.00 49.13 |
| MOTA | 3127 | CG | ARG B | 16 | | . 656 | 16.197 | 80.447 | 1.00 54.22 |
| ATOM | - | CD | ARG B | 16 | | . 858 | 15.624 | 79.751 | 1.00 55.13 |
| MOTA | 3128 3129 | NE | ARG B | 16 | 44 | .303 | 16.549 | 78.718 | 1.00 62.87 |
| MOTA | 3130 | CZ | ARG B | 16 | | .628 | 17.818 | 78.951 | 1.00 64.92 |
| MOTA | | NH1 | ARG B | 16 | | . 556 | 18.308 | 80.182 | 1.00 65.86 |
| ATOM | 3131 | NH2 | ARG B | 16 | | .022 | 18.600 | 77.954 | 1.00 67.15 |
| ATOM | 3132 | C | ARG B | 16 | | .093 | 13.531 | 82.728 | 1.00 42.97 |
| ATOM | 3133 3134 | 0 | ARG B | 16 | | .882 | 13.593 | 82.927 | 1.00 38.44 |
| MOTA | 3135 | N | TYR B | 17 | 41 | .949 | 13.056 | 83.628 | 1.00 39.36 |
| ATOM | 3136 | CA | TYR B | 17 | 41 | .494 | 12.637 | 84.945 | 1.00 37.67 |
| MOTA | 3137 | СВ | TYR B | 17 | | .500 | 11.679 | 85.584 | 1.00 31.69 |
| ATOM | 3138 | CG | TYR B | 17 | 42 | .413 | 10.250 | 85.087 | 1.00 28.00 |
| ATOM ATOM | 3139 | CD1 | | 17 | 42 | .530 | 9.944 | 83.732 | 1.00 22.89 1.00 21.42 |
| ATOM | 3140 | CE1 | | 17 | 42 | .502 | 8.618 | 83.287 | 1.00 21.42 |
| ATOM | 3141 | CD2 | | 17 | | .258 | 9.196 | 85.984 | 1.00 24.67 |
| ATOM | 3142 | CE2 | | 17 | | .229 | 7.873 | 85.556 | 1.00 27.13 |
| ATOM | 3143 | CZ | TYR B | 17 | | .355 | 7.587 | 84.210 | 1.00 27.13 |
| ATOM | 3144 | он | TYR B | 17 | | .371 | 6.271 | 83.796 85.765 | 1.00 38.94 |
| ATOM | 3145 | С | TYR B | 17 | | .377 | 13.927 | 85.391 | 1.00 39.65 |
| ATOM | 3146 | 0 | TYR B | 17 | | .947 | 14.951 | 86.891 | 1.00 41.27 |
| ATOM | 3147 | N | PRO B | 18 | | .647 | 13.893 | 87.462 | 1.00 43.62 |
| MOTA | 3148 | CD | PRO B | 18 | | .958 | 12.728 15.058 | 87.762 | 1.00 45.33 |
| MOTA | 3149 | CA | PRO B | 18 | | .448 | 14.473 | 88.928 | 1.00 44.09 |
| ATOM | 3150 | CB | PRO B | 18 | | 648 0.096 | 13.015 | 88.933 | 1.00 49.22 |
| ATOM | 3151 | CG | PRO B | 18 | | 1.096 | 15.809 | 88.221 | |
| MOTA | 3152 | С | PRO B | 18 | | 2.789 | 15.244 | 88.317 | 1.00 45.44 |
| ATOM | 3153 | 0 | PRO B | 18 19 | | 1.506 | 17.095 | 88.507 | 1.00 48.42 |
| MOTA | 3154 | N | LYS B | 19 | | 2.535 | 18.040 | 88.952 | 1.00 51.03 |
| MOTA | 3155 | CA | LYS B | 19 | | 1.873 | 19.122 | 89.814 | 1.00 56.35 |
| ATOM | 3156 | CB | LYS B | 19 | | 0.630 | 18.657 | 90.563 | 1.00 65.69 |
| ATOM | 3157 | CG CD | LYS B | 19 | | 0.894 | 17.441 | 91.423 | 1.00 68.96 |
| MOTA | 3158 3159 | CE | LYS B | 19 | | 9.602 | 16.882 | 91.999 | 1.00 71.85 |
| MOTA | 3160 | NZ | LYS B | 19 | 3: | 9.825 | 15.603 | 92.731 | 1.00 72.79 |
| MOTA MOTA | 3161 | C | LYS B | 19 | 4 | 3.830 | 17.593 | 89.639 | 1.00 48.62 1.00 49.04 |
| MOTA | 3162 | ō | LYS B | 19 | | 4.912 | 18.009 | 89.235 | 1.00 43.04 |
| MOTA | 3163 | N | ASN B | 20 | _ | 3.745 | 16.775 | 90.678 91.375 | 1.00 43.86 |
| MOTA | 3164 | CA | ASN B | 20 | | 4.957 | 16.356 | 92.890 | 1.00 45.92 |
| ATOM | 3165 | CB | ASN B | 20 | | 4.740 | | 93.355 | 1.00 49.44 |
| ATOM | 3166 | CG | ASN B | 20 | | 4.418 | | 93.138 | 1.00 47.72 |
| ATOM | 3167 | | 1 ASN B | 20 | | 5.194 | | 93.999 | 1.00 49.42 |
| MOTA | 3168 | ND: | | 20 | | 3.268 5.460 | | | 1.00 39.49 |
| MOTA | 3169 | Ç | ASN B | 20 | _ | 6.496 | | 91.494 | 1.00 38.24 |
| ATCM | 3170 | 0 | ASN B | 20 21 | | 4.729 | | 00 140 | 1.00 36.93 |
| ATOM | 3171 | N | HIS B | | | 5.091 | | 8 723 | 1.00 33.57 |
| MOTA | 3172 | | | | | 3.948 | | | 1.00 28.67 |
| ATOM | 3173 | | | | | 4.068 | 10.817 | 88.750 | |
| ATOM | 3174 | | | | | 4.779 | 10.076 | 87.867 | |
| ATOM | 3175 3176 | | 1 HIS B | | | 3.431 | | 89.578 | |
| ATOM | 3177 | | 1 HIS B | | 4 | 3.743 | 8.686 | | |
| ATOM | 3178 | | 2 HIS B | | | 4.560 | 8.755 | | |
| ATOM | 3179 | | HIS E | | | 6.348 | | | |
| MOTA MOTA | 3180 | | HIS B | | | 6.536 | | | |
| ATOM | 3181 | | PRO E | | | 7.225 | | | |
| ATOM | 3182 | | | 3 22 | | 17.187 | | | |
| ATOM | 3183 | - | | 3 22 | | 18.446 | | | |
| ATOM | 3184 | | | | | 19.05 | | | |
| ATCM | 3185 | | | | | 13.658 | | | |
| ATOM | 3186 | | PRO P | | | 48.17 | | | |
| ATCM | 318 | 7 0 | PRO I | | • | 48.989 | | | 7 1.00 24.47 |
| ATOM | 318 | | LEU ! | | | 47.03 | | _ | |
| ATOM | 318 | | A LEU | | | 46.68 45.93 | | _ | 3 1.00 22.18 |
| ATOM | 319 | | | B 23 | | 45.93. 46.76 | | - | |
| ATCM | 319 | 1 0 | G LEU | в 23 | | 40.70 | 0.03 | | |

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| | | | | | | 45 060 | 7.628 | 84.402 | 1.00 24.94 |
|-------|--------|-----|-------|-------|---|--------|--------|--------|------------|
| M | 3192 | | LEU B | 23 | | 45.868 | | | |
| M | 3193 | CD2 | LĘU B | 23 | | 47.805 | 8.905 | 83.446 | |
| | 3194 | | LEU B | 23 | | 45.891 | 12.638 | 84.367 | 1.00 27.95 |
| M | | - | | 23 | | 45.166 | 12.528 | 83.373 | 1.00 24.42 |
| М | 3195 | - | LEU B | | | | | 85.018 | 1.00 31.01 |
| M | 3196 | 7 | LYS B | 24 | | 46.011 | 13.793 | | |
| M | 3197 | | LYS B | 24 | | 45.261 | 14.946 | 84.530 | 1.00 29.40 |
| | - | | | 24 | | 44.934 | 15.923 | 85.665 | 1.00 33.03 |
| M | 3198 | - | LYS B | | | _ | 16.969 | 85.999 | 1.00 33.54 |
| M | 3199 | ÇG | LYS B | 24 | | 45.979 | | | |
| ·Μ | 3200 | CD | LYS B | 24 | | 47.300 | 16.397 | 86.422 | 1.00 39.10 |
| | 3201 | | LYS B | 24 | | 48.109 | 17.466 | 87.152 | 1.00 45.49 |
| M | | | | | | 48.224 | 18.737 | 86.380 | 1.00 45.95 |
| M | 3202 | | LYS B | 24 | | | | | 1.00 30.02 |
| M | 3203 | С | LYS B | 24 | | 46.039 | 15.653 | 83.425 | |
| M | 3204 | | LYS B | 24 | | 45.508 | 16.523 | 82.736 | 1.00 28.82 |
| | | | ILE B | 25 | | 47.298 | 15.262 | 83.246 | 1.00 25.93 |
| M | 3205 | N | | | | 48.139 | 15.858 | 82.212 | 1.00 29.48 |
| M | 3206 | CA | ILE B | 25 | | | | | 1.00 33.61 |
| M | 3207 | CB | ILE B | 25 | | 49.541 | 15.528 | 82.409 | |
|)M | 3208 | CG2 | ILE B | 25 | | 50.126 | 16.033 | 83.775 | 1.00 32.27 |
| | | CG1 | ILE B | 25 | | 49.851 | 14.014 | 82.263 | 1.00 28.17 |
| M | 3209 | | | | | 51.310 | 13.584 | 82.188 | 1.00 36.32 |
| M | 3210 | | ILE B | 25 | | | | 80.834 | 1.00 30.08 |
|)M | 3211 | С | ILE B | 25 | | 47.784 | 15.318 | | |
| M | 3212 | 0 | ILE B | 25 | | 47.263 | 14.210 | 80.704 | 1.00 25.37 |
| | 3213 | N | PRO B | 26 | | 48.064 | 16.101 | 79.783 | 1.00 29.19 |
| M | | | | | | 48.650 | 17.448 | 79.770 | 1.00 32.47 |
| MC | 3214 | CD | PRO B | 26 | | | | 78.413 | 1.00 29.52 |
| MC | 3215 | CA | PRO B | 26 | | 47.782 | 15.673 | | |
| MC | 3216 | CB | PRO B | 26 | | 48.103 | 16.921 | 77.593 | 1.00 29.84 |
| | 3217 | CG | PRO B | 26 | | 47.930 | 18.046 | 78.599 | 1.00 36.40 |
| MC | | | | | | 48.789 | 14.561 | 78.137 | 1.00 27.64 |
| MC | 3218 | С | PRO B | 26 | | | | 78.629 | 1.00 23.08 |
| MC | 3219 | 0 | PRO B | 26 | - | 49.920 | 14.620 | | |
| MC | 3220 | N | ARG B | 27 | | 48.403 | 13.557 | 77.360 | 1.00 23.09 |
| | | CA | ARG B | 27 | | 49.326 | 12.469 | 77.072 | 1.00 23.00 |
| MC | 3221 | | | | | 48.987 | 11.264 | 77.962 | 1.00 26.21 |
| MC | 3222 | CB | ARG B | 27 | | | | | 1.00 17.03 |
| MC | 3223 | CG | ARG B | 27 | | 49.101 | 11.617 | 79.449 | |
| MC | 3224 | CD | ARG B | 27 | | 48.663 | 10.507 | 80.416 | 1.00 26.83 |
| | | NE | ARG B | 27 | | 49.586 | 9.375 | 80.502 | 1.00 22.99 |
| MC | 3225 | | | | | 49.444 | 8.220 | 79.856 | 1.00 25.06 |
| MC | 3226 | CZ | ARG B | 27 | | | | 79.059 | 1.00 17.74 |
| MC | 3227 | NHl | ARG B | 27 | | 48.408 | 8.022 | _ | |
| DM | 3228 | NH2 | ARG B | 27 | | 50.336 | 7.253 | 80.027 | 1.00 23.38 |
| | | | ARG B | | | 49.329 | 12.097 | 75.595 | 1.00 22.54 |
| MC | 3229 - | | | | | 50.214 | 12.526 | 74.852 | 1.00 21.86 |
| MC | 3230 | O | ARG B | | | | | 75.148 | 1.00 20.64 |
| MC | 3231 | N | VAL E | 28 | | 48.352 | 11.318 | | |
| OM | 3232 | CA | VAL B | 28 | | 48.337 | 10.954 | 73.739 | 1.00 26.57 |
| | 3233 | СВ | VAL B | | | 47.242 | 9.917 | 73.424 | 1.00 30.92 |
| OM | | | | | | 47.195 | 9.645 | 71.925 | 1.00 27.04 |
| MO | 3234 | CG1 | VAL B | | | | | 74.172 | 1.00 25.45 |
| OM | 3235 | CG2 | VAL B | | | 47.535 | 8.616 | | |
| OM | 3236 | C | VAL B | 28 | | 48.150 | 12.189 | 72.866 | 1.00 28.02 |
| | 3037 | Э | VAL B | | | 48.780 | 12.311 | 71.808 | 1.00 30.88 |
| OM | - | | | | | 47.298 | 13.112 | 73.304 | 1.00 24.30 |
| OM | 3.38 | 7/ | SER B | | | | | 72.523 | 1.00 29.48 |
| OM | 3139 | CA | SER B | | | 47.082 | 14.326 | | |
| OM | 3240 | CB | SER B | 29 | | 45.939 | 15.169 | 73.110 | 1.00 31.72 |
| | 3241 | ЭG | SER 3 | | | 46.218 | 15.614 | 74.424 | 1.00 34.55 |
| MO | | | | | | 48.379 | 15.125 | 72.514 | 1.00 30.81 |
| OM | 3242 | С | SER B | | | | 15.820 | 71.545 | 1.00 28.85 |
| OM | 3243 | Э | SER B | | | 48.680 | | | 1.00 29.63 |
| 'OM | 3244 | N | LEU B | 30 | | 49.157 | 15.003 | 73.589 | 1.00 29.03 |
| | .3245 | CA | LEU 9 | | | 50.427 | 15.721 | 73.679 | 1.00 31.59 |
| 'OM | | | | | | 51.046 | 15.593 | 75.079 | 1.00 29.49 |
| MO' | 3246 | CB | LEU B | | | | 16.660 | 75.513 | 1.00 34.37 |
| OM | 3247 | CG | LEU B | | | 52.066 | | | 1.00 30.15 |
| 'OM | 3248 | CD1 | LEU B | 30 | | 52.937 | 16.083 | 76.610 | |
| | 3249 | CD2 | | | | 52.951 | 17.098 | 74.357 | 1.00 32.90 |
| MO' | | | | | | 51.371 | 15.085 | 72.672 | 1.00 25.90 |
| MO' | 3250 | 2 | LEU E | | | 52.5.2 | 15.777 | 71.913 | 1.00 25.10 |
| MO' | 3251 | Э | LEU E | | | 52.052 | | | |
| 'OM | 3252 | M | LEU B | 31 | | 51.404 | 13.756 | 72.675 | |
| | 3253 | CA | LEU E | | | 52.268 | 13.013 | 71.764 | 1.00 25.52 |
| MO | | | | | | 51.966 | 11.514 | 71.842 | 1.00 26.41 |
| CM | 3254 | CB | LEU E | | | 52.056 | 10.524 | 71.441 | 1.00 28.93 |
| CM | 3255 | CG | LEU E | | | 53.066 | | 71.042 | 1.00 23.69 |
| MO. | 3256 | CD1 | LEU E | 3 3 1 | | 52.425 | 9.198 | | |
| CM | 3257 | CD2 | LEU E | 3 3 1 | | 53.873 | 11.049 | 70.300 | 1.00 30.41 |
| . 641 | | | | | | | | | |

| | | _ | LEU 3 | 31 | | 52.010 | 13.489 | 70.335 | 1.00 25.38 |
|------|------|-------|-------|----------|---|------------------|------------------|--------|------------|
| ATOM | 3258 | _ | LEU 3 | 31 | | 52.940 | 13.851 | 69.614 | 1.00 21.03 |
| MOTA | 3259 | - | LEU B | 32 | | 50.741 | 13.481 | 69.933 | 1.00 21.27 |
| MOTA | 3260 | | | 32 | | 50.364 | 13.899 | 68.585 | 1.00 27.91 |
| ATOM | 3261 | | LEU 3 | 32 | | 48.841 | 13.798 | 68.408 | 1.00 26.60 |
| MOTA | 3262 | | LEU B | | | 48.195 | 12.419 | 68.614 | 1.00 27.30 |
| MOTA | 3263 | | LEU 3 | 32 | | 46.699 | 12.504 | 68.321 | 1.00 31.60 |
| MOTA | 3264 | CD1 - | | 32 | | 48.837 | 11.391 | 67.708 | 1.00 26.90 |
| ATOM | 3265 | | LEU 3 | 32 | | | 15.317 | 68.242 | 1.00 26.07 |
| MOTA | 3266 | - | TEO 3 | | | 50.835 | 15.533 | 67.205 | 1.00 22.45 |
| MOTA | 3267 | | LEU 3 | 32 | | 51.458 | 16.282 | 69.111 | 1.00 28.19 |
| MOTA | 3268 | N | ARG 3 | 33 | • | 50.545 | 17.660 | 68.865 | 1.00 31.77 |
| ATOM | 3269 | CA | ARG B | | | 50.962 | 18.601 | 69.930 | 1.00 34.22 |
| MOTA | 3270 | CB | ARG B | 33 | | 50.395 | 18.740 | 69.904 | 1.00 40.33 |
| MOTA | 3271 | CG | ARG 3 | | | 48.887 | 19.713 | 70.970 | 1.00 47.67 |
| ATOM | 3272 | CD | ARG B | | | 48.420 | 19.713 | 70.924 | 1.00 56.24 |
| ATOM | 3273 | ΝE | ARG B | | | 46.977 | 20.505 | 69.912 | 1.00 60.10 |
| MOTA | 3274 | CZ | ARG 3 | | | 46.330 | 20.929 | 68.845 | 1.00 63.11 |
| ATOM | 3275 | NH1 | ARG 3 | | | 46.997 | 20.652 | 69.965 | 1.00 63.81 |
| MOTA | 3276 | NH2 | ARG B | | | 45.011 52.476 | 17.791 | 68.852 | 1.00 30.12 |
| MOTA | 3277 | С | ARG 3 | | | 53.028 | 18.580 | 68.097 | 1.00 30.20 |
| MOTA | 3278 | 0 | ARG B | | | 53.147 | 17.012 | 69.694 | 1.00 30.70 |
| MOTA | 3279 | N | PHE 3 | | | 54.600 | 17.060 | 69.774 | 1.00 29.42 |
| MOTA | 3280 | CA | PHE B | | | | 16.176 | 70.920 | 1.00 30.46 |
| MOTA | 3281 | CB | PHE B | | | 55.096 | 16.358 | 71.248 | 1.00 28.56 |
| MOTA | 3282 | CG | PHE B | | | 56.556 | 17.515 | 71.885 | 1.00 26.92 |
| MOTA | 3283 | CD1 | PHE B | | | 57.001 | | 70.932 | 1.00 28.88 |
| MOTA | 3284 | CD2 | PHE B | | | 57.481 | 15.373 17.684 | 72.206 | 1.00 28.15 |
| MOTA | 3285 | | PHE E | | | 58.346 | 15.530 | 71.246 | 1.00 31.47 |
| MOTA | 3286 | CE2 | | | | 58.831 | 16.689 | 71.887 | 1.00 28.15 |
| MOTA | 3287 | CZ | PHE B | | | 59.265 | 16.583 | 68.460 | 1.00 33.78 |
| MOTA | 3288 | С | PHE E | | | 55.202 | 17.259 | 67.873 | 1.00 33.71 |
| MOTA | 3289 | 0 | PHE E | | | 56.049 | 15.413 | 67.999 | 1.00 28.65 |
| ATOM | 3290 | N | LYS | | | 54.770 | 14.880 | 66.753 | 1.00 34.33 |
| MOTA | 3291 | CA | LYS | | | 55.294 | 13.509 | 66.454 | 1.00 32.97 |
| MOTA | 3292 | CB | LYS 5 | _ | | 54.684 55.141 | 12.423 | 67.414 | 1.00 34.93 |
| ATOM | 3293 | CG | LYS | | | 54.580 | 11.066 | 67.047 | 1.00 41.43 |
| ATOM | 3294 | CD | LYS | | | 53.070 | 11.004 | 67.205 | 1.00 44.04 |
| MOTA | 3295 | CE | LYS | | | 52.335 | 11.984 | 66.345 | 1.00 60.09 |
| ATOM | 3296 | NZ | LYS | | | 55.015 | 15.842 | 65.608 | 1.00 35.78 |
| ATOM | 3297 | C | LYS | | | 55.869 | 16.061 | 64.752 | 1.00 33.39 |
| MOTA | 3298 | 0 | LYS | | | 53.823 | 16.426 | 65.602 | 1.00 32.32 |
| MOTA | 3299 | N | ASP ! | | | 53.468 | 17.365 | 64.552 | 1.00 36.31 |
| ATOM | 3300 | CA | ASP | | | 52.015 | 17.800 | 64.698 | 1.00 42.56 |
| MOTA | 3301 | CB | ASP : | | | 51.617 | 18.822 | 63.661 | 1.00 43.03 |
| ATOM | 3302 | CG | ASP : | | | 51.812 | 18.544 | 62.461 | 1.00 79.17 |
| MOTA | 3303 | OD1 | | | | 51.111 | 19.897 | 64.043 | 1.00 .4.34 |
| MOTA | 3304 | | ASP | | | 54.371 | 18.590 | 64.578 | 1.00 6.14 |
| ATOM | 3305 | С | ASP | | | 54.764 | 19.099 | 63.534 | 1.00 32.40 |
| MOTA | 3306 | 0 | ASP | | | 54.694 | 19.061 | 65.777 | 1.00 34.80 |
| MOTA | 3307 | N | ALA | | | 55.554 | 20.226 | 65.924 | |
| ATOM | 3308 | CA | ALA | | | 55.599 | 20.659 | 67.383 | 1.00 38.54 |
| ATOM | 3309 | CB | ALA | | | 56.959 | 19.901 | 65.429 | 1.00 37.66 |
| MOTA | 3310 | С | ALA | | | 57.675 | 20.776 | | 1.00 30.56 |
| MOTA | 3311 | 0 | ALA | | | 57.346 | 18.635 | 65.541 | 1.00 37.42 |
| ATOM | 3312 | N | | 38 | | | 18.192 | 65.107 | 1.00 36.25 |
| MOTA | 3313 | CA | MET | | | 58.670 | 17.059 | 66.013 | 1.00 36.44 |
| ATOM | 3314 | CB | | 38 38 | | 59.158 | 17.438 | 67.474 | 1.00 37.68 |
| ATOM | 3315 | CG | | 38 | | 59.341 | | 67.784 | |
| MOTA | 3316 | SD | | 3 38 | | 60.841 | 18.391 17.228 | | |
| ATOM | 3317 | CE | | 38 | | 62.093 | | | |
| ATOM | 3318 | С | MET | | | 58.639 | 17.690 | | |
| ATOM | 3319 | | MET | | | 59.659 | 17.262 | | |
| ATOM | 3320 | | ASN | | | 57.470 | | | |
| ATOM | 3321 | CA | | | | 57.321 | 17.262 | | |
| ATOM | 3322 | CB | | | | 58.156 | | | |
| ATOM | 3323 | | ASN | B 39 | | 57.670 | 19.543 | | |
| | | | | | | | | | |

| | | | | | | | 10 001 | 60.212 | 1.00 48.78 |
|-------|------|-----|---------|------|---|--------|--------|----------|---|
| ATOM | 3324 | OD1 | ASN B | 39 | | 56.524 | 19.801 | | 1.00 46.52 |
| ATOM | 3325 | ND2 | ASN B | 39 | | 58.540 | 20.486 | 60.933 | 1.00 39.12 |
| ATOM | 3326 | С | ASN B | 39 | | 57.759 | 15.804 | 61.569 | |
| | 3327 | ō | ASN B | 39 | | 58.465 | 15.416 | 60.639 | 1.00 35.75 |
| ATOM | | | LEU B | 40 | | 57.332 | 14.997 | 62.535 | 1.00 34.64 |
| MOTA | 3328 | N | | 40 | | 57.700 | 13.590 | 62.556 | 1.00 35.10 |
| MOTA | 3329 | ÇA | LEU B | | | 58.347 | 13.248 | 63.898 | 1.00 35.97 |
| ATOM | 3330 | CB | LEU B | 40 | | | 14.073 | 64.227 | 1.00 36.21 |
| ATOM | 3331 | CG | LEU B | 40 | | 59.595 | | 65.573 | 1.00 36.57 |
| MOTA | 3332 | CD1 | LEU B | 40 | | 60.148 | 13.648 | | 1.00 36.79 |
| MOTA | 3333 | CD2 | LEU B | 40 | | 60.646 | 13.880 | 63.145 | |
| MOTA | 3334 | С | LEU B | 40 | | 56.549 | 12.626 | 62.264 | |
| | 3335 | ō | LEU B | 40 | | 56.637 | 11.438 | 62.573 | 1.00 39.15 |
| MOTA | 3336 | N | ILE B | 41 | • | 55.476 | 13.131 | 61.663 | 1.00 36.79 |
| MOTA | | CA | ILE B | 41 | | 54.340 | 12.290 | 61.314 | 1.00 35.42 |
| MOTA | 3337 | | ILE B | 41 | | 53.445 | 11.991 | 62.536 | 1.00 35.21 |
| MOTA | 3338 | CB | | 41 | | 52.793 | 13.271 | 63.047 | 1.00 31.89 |
| MOTA | 3339 | CG2 | | | | 52.367 | 10.980 | 62.141 | 1.00 32.68 |
| ATOM | 3340 | CG1 | | 41 | | 51.470 | 10.550 | 63.285 | 1.00 36.46 |
| ATOM | 3341 | CD1 | | 41 | | 53.492 | 12.937 | 60.229 | 1.00 37.52 |
| MOTA | 3342 | С | ILE B | 41 | | | 14.157 | 60.183 | 1.00 40.24 |
| MOTA | 3343 | 0 | ILE B | 41 | | 53.352 | | 59.345 | 1.00 39.55 |
| ATOM | 3344 | N | ASP B | 42 | | 52.943 | 12.114 | 58.273 | 1.00 45.30 |
| MOTA | 3345 | CA | ASP B | 42 | | 52.094 | 12.615 | | 1.00 45.93 |
| ATOM | 3346 | CB | ASP B | 42 | | 52.569 | 12.119 | 56.901 | |
| ATOM | 3347 | CG | ASP B | 42 | | 53.972 | 12.584 | 56.564 | |
| | 3348 | OD1 | | 42 | | 54.244 | 13.799 | 56.686 | 1.00 46.60 |
| MOTA | 3349 | OD2 | | 42 | | 54.797 | 11.736 | 56.162 | 1.00 45.16 |
| ATOM | 3350 | C | ASP B | 42 | | 50.677 | 12.134 | 58.524 | 1.00 45.15 |
| ATOM | | Ö | ASP B | 42 | | 50.467 | 11.051 | 59.069 | 1.00 47.06 |
| MOTA | 3351 | N | GLU B | 43 | | 49.707 | 12.944 | 58.121 | 1.00 48.13 |
| MOTA | 3352 | | GLU B | 43 | | 48.303 | 12.618 | 58.312 | 1.00 50.50 |
| MOTA | 3353 | CA | GLU B | 43 | • | 47.441 | 13.637 | 57.571 | 1.00 53.54 |
| ATOM | 3354 | CB | | 43 | | 45,961 | 13.505 | 57.840 | 1.00 59.52 |
| MOTA | 3355 | CG | GLU B | 43 | | 45.155 | 14.518 | 57.065 | 1.00 64.03 |
| ATOM | 3356 | CD | GLU B | 43 | | 43.914 | 14.535 | 57.215 | 1.00 68.54 |
| MOTA | 3357 | OE1 | | | | 45.765 | 15.298 | 56.301 | 1.00 66.95 |
| MOTA | 3358 | OE2 | | 43 | | 47.972 | 11.205 | 57.836 | 1.00 47.81 |
| MOTA | 3359 | C | GLU B | 43 | | 47.092 | 10.547 | 58.390 | 1.00 49.67 |
| MOTA | 3360 | 0 | GLU B | 43 | | 48.690 | 10.744 | 56.817 | 1.00 46.21 |
| ATOM | 3361 | N | LYS B | 44 | | 48.484 | 9.409 | 56.251 | 1.00 48.28 |
| MOTA | 3362 | CA | LYS B | 44 | | 49.207 | 9.311 | 54.894 | 1.00 49.96 |
| MOTA | 3363 | CB | LYS B | 44 | | 49.639 | 7.903 | 54.470 | 1.00 52.18 |
| ATOM | 3364 | CG | LYS B | 44 | | 50.970 | 7.532 | 55.127 | 1.00 61.03 |
| MOTA | 3365 | CD | LYS B | 44 | | | 6.095 | 54.844 | 1.00 62.80 |
| ATOM | 3366 | CE | LYS B | 44 | | 51.399 | 5.098 | 55.510 | 1.00 65.34 |
| MOTA | 3367 | NZ | LYS B | 44 | | 50.511 | | 57.161 | 1.00 45.92 |
| MOTA | 3368 | С | LYS B | 44 | | 48.899 | 8.249 | 57.009 | 1.00 41.30 |
| ATOM | 3369 | 0 | LYS B | 44 | | 48.418 | 7.127 | | 1.00 42.18 |
| ATOM | 3370 | N | GLL B | 45 | | 49.797 | 8.517 | 58.100 | 1.00 38.41 |
| ATOM | 3371 | CA | GLU B | 45 | | 50.268 | 7.486 | . 59.014 | 1.00 33.73 |
| ATOM | 3372 | СВ | GLU B | 45 | | 51.684 | 7.812 | 59.468 | 1.00 37.58 |
| ATOM | 3373 | CG | GLU B | 45 | | 52.694 | 7.887 | 58.351 | 1.00 34.34 |
| ATOM | 3374 | CD | GLU B | | | 53.998 | 8.504 | 58.813 | 1.00 34.34 |
| | | | 1 GLU B | | | 53.997 | 9.699 | 59.176 | 1.00 30.04 |
| ATOM | 3376 | OE | | | | 55.020 | 7.799 | 58.821 | 1.00 33.37 |
| MOTA | 3377 | C C | GLU B | | | 49.368 | 7.403 | 60.238 | 1.00 36.86 |
| ATOM | | 0 | GLU B | | | 49.461 | 6.462 | 61.032 | 1.00 34.98 |
| ATOM | 3378 | | | | | 48.489 | 8.386 | 60.386 | 1.00 30.86 |
| ATCM | 3379 | 14 | LEU B | | | 47.608 | | 61.545 | 1.00 30.65 |
| MOTA | 3380 | CA | | _ | | 47.501 | | 62.019 | |
| ATOM | 3381 | CE | | | | 46.642 | | 63.250 | 1.00 34.76 |
| ATOM | 3382 | | | | | 47.189 | | | 1.00 32.24 |
| ATOM | 3383 | | 1 LEU E | | | - | | | 1.00 33.94 |
| ATCM | 3384 | CD | | | | 46.639 | | | 1.00 31.36 |
| ATOM | 3385 | | LEU E | | | 46.212 | | | 1.00 31.78 |
| ATOM | 3386 | 0 | LEU E | | | 45.530 | | | |
| ATOM | 3387 | | ILE E | | | 45.801 | | | |
| ATCM | 3388 | | ILE E | 3 47 | | 44.479 | | | |
| ATOM | 3389 | | ILE F | 3 47 | | 44.564 | 4.802 | , | , <u>,</u> ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| 41011 | · | | | | | | | | |

| 3 mov | 3390 | CG2 | ILE B | 47 | 43.161 | 4.205 | 62.407 | 1.00 28.80 |
|-------|------|-----|-------|------|--------|--------|--------|-------------|
| ATOM | - | | | | 45.266 | 4.230 | 61.028 | 1.00 29.42 |
| MOTA | 3391 | CG1 | ILE B | 47 | | | | 1.00 31.12 |
| | 3392 | CD1 | ILE B | 47 | 45.419 | 2.722 | 61.054 | |
| ATOM | - | - | | | 43.659 | 6.875 | 63.303 | 1.00 32.22 |
| ATOM | 3393 | С | ILE B | 47 | | | 64.461 | 1.00 31.17 |
| ATOM | 3394 | 0 | ILE B | 47 | 44.063 | 6.755 | | |
| | - | | | 48 | 42.514 | 7.475 | 62.999 | 1.00 28.39 |
| ATOM | 3395 | 11 | LYS B | | 42.511 | | 64.340 | 1.00 32.37 |
| MOTA | 3396 | CA | LYS B | 48 | 41.662 | 8.037 | | |
| | | CB | LYS B | 48 | 40.517 | 8.840 | 63.414 | 1.00 36.32 |
| ATOM | 3397 | | | | 39.607 | 9.514 | 64.430 | 1.00 43.08 |
| MOTA | 3398 | CG | LYS B | 48 | | | _ | 1.00 44.38 |
| ATOM | 3399 | CD | LYS B | 48 | 38.535 | 10.361 | 63.747 | |
| | | | LYS B | 48 | 37.657 | 11.074 | 64.768 | 1.00 45.91 |
| MOTA | 3400 | CE | _ | | | 11.991 | 65.643 | 1.00 42.66 |
| ATOM | 3401 | ΝZ | LYS B | 48 | 38.451 | | | 1.00 31.08 |
| MOTA | 3402 | С | LYS B | 48 | 41.095 | 6.943 | 64.937 | |
| | | | LYS B | 48 | 40.524 | 5.962 | 64.457 | 1.00 26.24 |
| ATOM | 3403 | 0 | | | 41.260 | 7.121 | 66.244 | 1.00 27.89 |
| ATOM | 3404 | N | SER B | 49 | | | | 1.00 25.17 |
| ATOM | 3405 | CA | SER B | 49 | 40.770 | 6.168 | 67.232 | |
| | - | | SER B | 49 | 41.146 | 6.639 | 68.642 | 1.00 24.41 |
| ATOM | 3406 | CB | | | 42.539 | 6.858 | 68.777 | 1.00 31.79 |
| MOTA | 3407 | OG | SER B | 49 | | | 67 160 | 1.00 29.07 |
| | 3408 | С | SER B | 49 | 39.248 | 6.054 | 67.160 | 1.00 25.07 |
| MOTA | | | SER B | | 38.565 | 7.034 | 66.879 | 1.00 28.47 |
| MOTA | 3409 | 0 | | | 38.723 | 4.859 | 67.409 | 1.00 26.13 |
| ATOM | 3410 | N | ARG B | | | _ | | 1.00 24.24 |
| | 3411 | CA | ARG B | 50 | 37.278 | 4.658 | 67.430 | |
| MOTA | | | ARG B | | 36.810 | 3.700 | 66.323 | 1.00 25.03 |
| MOTA | 3412 | CB | | | 37.231 | 2.233 | 66.507 | 1.00 26.54 |
| ATOM | 3413 | CG | ARG B | | | | 65.452 | 1.00 26.21 |
| ATOM | 3414 | CD | ARG B | 50 | 36.570 | 1.340 | | |
| | | | ARG B | | 37.006 | -0.058 | 65.504 | 1.00 25.13 |
| MOTA | 3415 | NE | | | 36.700 | -0.924 | 66.468 | 1.00 26.09 |
| ATOM | 3416 | CZ | ARG B | | | 0.524 | 67.497 | 1.00 23.42 |
| ATOM | 3417 | NH1 | ARG B | 50 | 35.941 | -0.558 | | |
| | | NH2 | | | 37.157 | -2.168 | 66.402 | 1.00 23.91 |
| MOTA | 3418 | | | | 36.937 | 4.037 | 68.775 | 1.00 23.83 |
| ATOM | 3419 | C | ARG B | | | | 69.403 | 1.00 21.60 |
| ATOM | 3420 | 0 | ARG E | 50 | 37.782 | 3.392 | | |
| | 3421 | N | PRO E | | 35.700 | 4.223 | 69.243 | 1.00 22.99 |
| MOTA | | | | | 34.554 | 4.962 | 68.688 | 1.00 25.09 |
| ATOM | 3422 | CD | PRO E | | | | 70.530 | 1.00 25.48 |
| ATOM | 3423 | CA | PRO E | 3 51 | 35.338 | 3.628 | | 1.00 26.32 |
| | 3424 | CB. | PRO E | | 33.949 | 4.217 | 70.802 | 1.00 26.32 |
| MOTA | | | | | 33.936 | 5.503 | 69.953 | 1.00 28.65 |
| MOTA | 3425 | CG | PRO E | | | 2.118 | 70.325 | 1.00 26.73 |
| ATOM | 3426 | С | PRO E | 3 51 | 35.264 | | | 1.00 18.87 |
| | 3427 | 0 | PRO E | 3 51 | 35.142 | 1.646 | 69.194 | |
| ATOM | | | ALA I | | 35.355 | 1.359 | 71.408 | 1.00 23.64 |
| MOTA | 3428 | N | | | 35.237 | -0.083 | 71.291 | 1.00 23.27 |
| ATOM | 3429 | ÇÀ | ALA E | 3 52 | | | _ | 1.00 26.31 |
| ATOM | 3430 | CB | ALA F | 3 52 | 35.811 | -0.757 | 72.521 | |
| | | c | ALA E | | 33.733 | -0.324 | 71.223 | 1.00 25.25 |
| ATOM | 3431 | | | | 32.950 | 0.515 | 71.677 | 1.00 22.78 |
| ATOM | 3432 | 0 | ALA E | | | | 70.651 | 1.00 22.77 |
| ATOM | 3433 | N | THR I | 3 53 | 33.321 | -1.447 | | |
| | | CA | THR I | | 31.900 | -1.760 | 70.596 | 1.00 26.90 |
| MOTA | 3434 | | | | 31.567 | -2.732 | 69.456 | 1.00 30.00 |
| ATOM | 3435 | CB | THR | | | 2 050 | 69.642 | 1.00 25.59 |
| MOTA | 3436 | OG: | THR I | B 53 | 32.305 | -3.950 | | 1 00 23 33 |
| | 3437 | CG: | | | 31.917 | -2.117 | 68.103 | 1.00 23.33 |
| MOTA | | | | | 31.579 | -2.445 | 71.916 | 1.00 30.41 |
| ATOM | 3438 | С | THR : | | | | 72.609 | 1.00 26.13 |
| MOTA | 3439 | 0 | THR : | B 53 | 32.484 | -2.917 | | |
| | 3440 | N | LYS 1 | B 54 | 30.300 | -2.504 | 72.268 | |
| MOTA | | | | | 29.909 | -3.140 | 73.514 | .1.00 30.24 |
| MOTA | 3441 | CA | LYS | | | -3.027 | 73.720 | 1.00 32.78 |
| MOTA | 3442 | CB | LYS | B 54 | 28.396 | | | 1.00 34.85 |
| | 3443 | CG | LYS | B 54 | 27.947 | -3.351 | 75.131 | 1.00 34.03 |
| MOTA | | | | | 26.445 | -3.204 | 75.268 | 1.00 41.13 |
| MOTA | 3444 | CD | LYS | | | -3.366 | 76.709 | 1.00 43.39 |
| ATOM | 3445 | CE | LYS | | 26.008 | | | |
| | 3446 | NZ | LYS | 3 54 | 26.464 | -2.257 | 77.582 | 1 00 20 20 |
| ATOM | | | LYS | _ | 30.329 | -4.603 | 73.442 | |
| ATOM | 3447 | C | | | 30.779 | | 74.430 | 1.00 26.71 |
| ATOM | 3448 | ၁ | LYS | | | | 72.256 | |
| | 3449 | N | GLU | 3 55 | 30.196 | | 74.430 | |
| ATOM | | | | | 30.577 | -6.577 | 72.032 | |
| ATOM | 3450 | | | | 30.288 | | 70.579 | 1.00 24.82 |
| ATCM | 3451 | CB | | | | | | |
| ATOM | 3452 | | GLU | | 30.671 | | | |
| | 3453 | | | | 30.453 | -8.737 | 68.767 | |
| ATOM | | | | | 30.638 | | 68.394 | 1.00 41.24 |
| ATOM | 3454 | | 1 GLU | _ | | | | |
| 2 TOM | 3455 | OE | 2 GLU | B 55 | 30.101 | -,.633 | | - |

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72.345
                                                             1.00 25.82
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                                  32.066
                  GLU B
                          55
       3456
ATOM
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ATOM
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                  GLU B
              N
       3458
ATOM
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                                                    72.093
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              CA
                  GLU B
       3459
ATOM
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              CB
                  GLU B
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ATOM
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                  GLU B
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              CG
ATOM-
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              CD
                  GLU B
       3462
MOTA
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              OE1 GLU B
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ATOM
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                                                    67.959
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              OE2 GLU B
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ATOM
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                  GLU B
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       3465
              С
MOTA
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                  GLU B
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ATOM
                                                             1.00 24.52
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                                   33.996
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       3467
                  LEU B
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ATOM
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                                                             1.00 27.34
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                          57
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MOTA
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                                                             1.00 22.79
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              CD1 LEU B
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        3471
MOTA
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              CD2 LEU B
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        3472
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        3473
              С
ATOM
                                                             1.00 24.06
                                                     77.396
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                   LEU B
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ATOM
                                                             1.00 23.35
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                   LEU B
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ATOM
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MOTA
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        3477
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ATOM
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                   LEU B
              CG
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                           58
              CD1 LEU
                       В
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ATOM
                                                              1.00 33.44
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              CD2 LEU B
        3480
 MOTA
                                                              1.00 24.59
                                                     76.446
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               С
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 MOTA
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        3482
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                                                              1.00 21.64
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                   LEU B
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                                                              1.00 24.24
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               CG
                   LEU B
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 MOTA
                                                              1.00 24.25
                                                     71.975
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               CD1 LEU B
        3487
 ATOM
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               CD2 LEU B
        3488
 MOTA
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                                                              1.00 19.39
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                   LEU B
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 MOTA
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 ATOM
                                                              1.00 23.08
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                                                              1.00 18.22
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                   PHE B
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                                                              1.00 21.72
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                   PHE B
               CG
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                                                              1.00 19.23
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         3495
                                                              1.00 17.75
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                                                      81.048
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                                    38.757
               CD2 PHE B
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 MOTA
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 STOM
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               CD2 HIS B
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         3506
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  ATOM
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                        В
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                                                               1.00 28.04
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                                                               1.00 25.25
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  STOM
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  ATOM
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                CB
                     GLU B
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ATCM

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 234567890123456789000000000000000000000000000000000000 | CD 12 CD | THR B THR B LEU B LEU B LEU B LEU B | 69 70 70 70 | 25.213 25.213 25.213 25.213 24.361 25.292 27.436 27.272 27.010 26.887 28.022 29.128 27.768 29.128 27.768 29.332 30.420 31.751 32.949 33.033 34.135 35.172 30.329 30.335 30.339 30.308 30.208 | 1.702 2.729 2.122 1.231 0.786 2.000 3.764 4.966 3.290 4.181 3.371 | 80.432 79.303 80.260 80.291 81.940 81.848 82.363 82.363 82.580 81.341 80.220 83.513 83.448 84.568 85.696 86.891 87.396 88.002 85.661 84.519 84.5519 85.661 | 1.00 22.90 1.00 25.91 1.00 28.47 1.00 25.13 1.00 21.32 1.00 22.33 1.00 22.57 1.00 23.20 1.00 23.02 1.00 19.62 1.00 25.87 1.00 24.80 1.00 30.37 |
|--|--|--|-------------------------------------|----------------------|--|---|--|--|
| | | Ç | LEU B | 69 | 30.036 | 3.764 | | |
| ATOM | | | | | | 3.290 | 82.294 | 1.00 19.62 |
| | | | | 70 | 28.449 | 4.181 | | |
| | 3581 | CB. | | _ | 27.660 | | | 1.00 30.37 |
| ATOM | 3582 3583 | | | | 27.592 | 1.599 | 78.227 | 1.00 30.35 |
| atom atom | 3584 | | MET B | 70 | 26.922 | 2.986 | | 1.00 28.82 |
| ATOM | 3585 | 5 C | MET B | | 27.489 27.391 | 5.062 L 6.273 | 82.009 | 1.00 24.09 |
| ATOM | 3586 | | MET E | | 26.786 | | | |
| ATOM | 3587 | 7 N | GLU E | , , , | 201 | | | |
| | | | | | | | | |

| | | | | | | , | | | • |
|--------------|--------------|----------|--------|----------|---|------------------|------------------|------------------|--------------------------|
| АТОМ | 3588 | CA | GLU B | 71 | | 25.837 | 5.207 | 84.008 | 1.00 27.45 1.00 30.70 |
| ATOM | 3589° | CB | GLU B | 71 | | 25.014 | 4.268 | 84.889 | 1.00 33.70 |
| ATOM | 3590 | | GLU B | 71 | | 24.072 | 5.005 | 85.832 | 1.00 37.51 |
| ATOM | 3591 | | GLU B | 71 | | 23.044 | 5.867 | 85.096 85.773 | 1.00 35.47 |
| MOTA | 3592 | | GLU B | 71 | | 22.333 | 6.638 | 83.849 | 1.00 31.03 |
| ATOM | 3593 | OE2 | GLU B | 71 | | 22.934 | 5.769 | 84.887 | 1.00 29.15 |
| ATOM | 3594 | C | GLU B | 71 | | 26.559 | 6.209 | 85.035 | 1.00 23.96 |
| ATOM | 3595 | 0 | GLU B | 71 | | 26.115 | 7.341 | 85.481 | 1.00 27.76 |
| ATOM | 3596 | N | ALA B. | | | 27.671 | 5.781 6.662 | 86.340 | 1.00 27.58 |
| MOTA | 3597 | CA | ALA B | 72 | | 28.454 29.663 | 5.920 | 86.909 | 1.00 23.24 |
| ATOM | 3598 | CB | ALA B | 72 | | 28.924 | 7.886 | 85.563 | 1.00 28.07 |
| MOTA | 3599 | C | ALA B | 72 72 | | 28.895 | 8.999 | 86.079 | 1.00 23.22 |
| MOTA | 3600 | 0 | ALA B | | | 29.356 | 7.684 | 84.322 | 1.00 26.40 |
| MOTA | 3601 | N. | GLU B | | | 29.846 | 8.801 | 83.529 | 1.00 29.06 |
| ATOM | 3602 3603 | CA CB | GLU B | | | 30.658 | 8.314 | 82.325 | 1.00 29.48 |
| ATOM | 3604 | CG | GLU B | | | 31.162 | 9.466 | 81.443 | 1.00 31.00 |
| MOTA MOTA | 3605 | CD | GLU B | | | 31.938 | 9.009 | 80.216 | 1.00 34.37 |
| ATOM | 3606 | | GLU B | | | 33.059 | 8.461 | 80.356 | 1.00 28.41 1.00 30.59 |
| ATOM | 3607 | OE2 | GLU B | 73 | | 31.419 | 9.203 | 79.100 | 1.00 30.59 1.00 31.92 |
| ATOM | 3608 | С | GLU B | | | 28.744 | 9.734 | 83.045 83.104 | 1.00 35.69 |
| MOTA | 3609 | 0 | GLU B | | | 28.894 | 10.951 | 83.104 | 1.00 33.53 |
| ATOM | 3610 | N | ARG B | | | 27.633 | 9.186 10.067 | 82.081 | 1.00 38.64 |
| MOTA | 3611 | CA | ARG B | | | 26.583 25.456 | 9.280 | 81.403 | 1.00 39.90 |
| ATOM | 3612 | CB | ARG B | | | 24.448 | 8.706 | 82.363 | 1.00 46.67 |
| MOTA | 3613 | CG | ARG B | | | 23.174 | 8.311 | 81.646 | 1.00 47.53 |
| MOTA | 3614 | CD | ARG E | | | 22.076 | 8.153 | 82.594 | 1.00 55.58 |
| ATOM | 3615 3616 | NE CZ | ARG E | | | 21.609 | 9.136 | 83.362 | 1.00 56.04 |
| MOTA | 3617 | NH1 | | | | 22.142 | 10.351 | 83.297 | 1.00 58.93 |
| ATOM | 3618 | NH2 | | | | 20.601 | 8.910 | 84.192 | 1.00 53.62 |
| MOTA MOTA | 3619 | С | ARG E | | | 26.008 | 10.914 | 83.222 | 1.00 35.84 1.00 29.44 |
| MOTA | 3620 | 0 | ARG E | 3 74 | | 25.778 | 12.107 | 83.048 | 1.00 23.44 |
| ATOM | 3621 | Ŋ | SER E | | | 25.794 | 10.302 11.014 | 84.386 85.539 | 1.00 31.99 |
| MOTA | 3622 | CA | SER E | | | 25.243 | 10.038 | 86.510 | 1.00 34.47 |
| MOTA | 3623 | CB | SER F | | | 24.592 25.581 | 9.228 | 87.123 | 1.00 34.33 |
| MOTA | 3624 | QG | SER I | | | 26.339 | 11.754 | 86.288 | 1.00 35.42 |
| ATOM | 3625 | С 0 | SER I | _ | | 26.060 | 12.555 | 87.180 | 1.00 33.45 |
| MOTA | 3626 3627 | N | GLN I | | _ | 27.584 | 11.473 | 85.922 | 1.00 33.25 |
| ATOM | 3628 | CA | GLN I | - | | 28.739 | 12.082 | 86.565 | 1.00 35.61 |
| MOTA MOTA | 3629 | CE | GLN I | | | 28.818 | 13.572 | 86.241 | 1.00 30.11 |
| ATOM | 3630 | CG | GLN I | | | 30.216 | 14.112 | 86.390 | 1.00 39.13 1.00 33.54 |
| ATOM | 3631 | CD | GLN | | | 31.124 | 13.681 | 85.248 84.761 | 1.00 33.34 |
| ATOM | 3632 | OE | L GLN | | | 31.052 | 12.546 | 84.827 | 1.00 40.93 |
| ATOM | 3633 | | GLN | | | 31.995 28.624 | 14 583 11 892 | 88.079 | 1.00 37.88 |
| ATOM | 3634 | Ç | GLN | | | 28.901 | 12 308 | 88.858 | 1.00 32.74 |
| ATOM | 3635 | 0 | GLN | | | 28.209 | 10.697 | 88.488 | 1.00 34.72 |
| ATOM | 3636 | Я | SER | | | 28.047 | 10.382 | 89.901 | 1.00 37.07 |
| ATOM | 3637 | CA | SER | | | 26.635 | 10.738 | 90.371 | |
| ATOM | 3638 | CB CG | SER | | | 25.678 | 9.941 | 89.688 | |
| MOTA | 3639 3640 | | SER | | | 28.265 | 8.897 | 90.112 | |
| ATOM ATOM | 3641 | | SER | | | 28.177 | 8.108 | 89.173 | |
| MOTA | 3642 | | VAL | | | 28.528 | 8.518 | 91.355 | 1.00 33.03 1.00 33.41 |
| ATOM | 3643 | | '/AL | | | 28.753 | 7.124 | | |
| ATOM | 3644 | | VAL | в 78 | | 29.742 | 6.979 | | |
| ATOM | 3645 | | | | | 29.955 | 5.499 | | |
| ATOM | 3646 | CG | | | | 31.055 | 7.658 | | 4 00 |
| ATOM | 3647 | C | VAL | | | 27.461 | 6.431 6.703 | | 1.00 28.25 |
| ATOM | 3648 | | VAL | B 78 | | 26.897 26.971 | 5.521 | | 1.00 36.73 |
| ATOM | 3649 | | PRO | | | 27.532 | 5.114 | | 1.00 37.44 |
| ATOM | 3650 | | | | | 25.738 | 4.779 | | 1.00 38.33 |
| ATOM | 3651 | | | | | 25.668 | 3.826 | 90.301 | 1.00 38.68 |
| MOTA | 3652 | | | _ | | 26.293 | 4.664 | | 1.00 37.41 |
| ATOM | 3653 | , (3 | PRO | , | | | | | |
| | | | | | | | | | |

| ATOM ATOM | 3654 3655 3656 | Ō | | B B B | 79 79 80 | 25.788 26.854 24.623 | 4.046 3.648 3.881 | 92.834 93.298 93.448 | 1.00 36.92 1.00 33.03 1.00 38.43 |
|----------------|----------------------|----------|--------------|-------------|----------------|----------------------------|-------------------------|----------------------------|--|
| ATOM ATOM | 3657 | | | В | 80 | 24.482 | 3.206 | 94.736 | 1.00 39.73 1.00 43.33 |
| ATOM | 3658 | СВ | | В | 80 | 23.003 | 2.871 2.129 | 94.967 96.262 | 1.00 44.60 |
| ATOM | 3659 | CG | LYS | | 80 | 22.679 21.198 | 1.742 | 96.287 | 1.00 48.09 |
| MOTA | 3660 | CD | | В | 80 80 | 20.805 | 1.014 | 97.559 | 1.00 50.12 |
| MOTA | 3661 3662 | CE NZ | LYS LYS | | 80 | 20.932 | 1.890 | 98.760 | 1.00 53.16 |
| MOTA MOTA | 3663 | C | LYS | | 80 | 25.315 | 1.928 | 94.854 | 1.00 40.35 1.00 36.67 |
| ATOM MOTA | 3664 | Ō | LYS | | 80 | 25.181 | 1.011 | 94.047 95.869 | 1.00 38.26 |
| MOTA | 3665 | N | GLY | | 81 | 26.173 26.996 | 1.880 0.709 | 96.104 | 1.00 34.69 |
| MOTA | 3666 | CA | GLY | | 81 | 28.066 | 0.407 | 95.071 | 1.00 34.63 |
| MOTA | 3667 | С 0 | GLY GLY | | 81 81 | 28.861 | -0.513 | 95.255 | 1.00 33.92 |
| MOTA | 3668 3669 | И | ALA | | 82 | 28.100 | 1.178 | 93.992- | 1.00 31.26 |
| MOTA MOTA | 3670 | CA | ALA | | 82 | 29.082 | 0.963 | 92.936 91.751 | 1.00 34.88 1.00 23.13 |
| ATOM | 3671 | CB | ALA | | 82 | 28.755 | 1.848 1.223 | 93.405 | 1.00 36.85 |
| MOTA | 3672 | C | ALA | | 82 | 30.517 31.461 | 0.580 | 92.945 | 1.00 32.17 |
| MOTA | 3673 | 0 | ALA ARG | | 82 83 | 30.677 | 2.168 | 94.323 | 1.00 36.52 |
| MOTA | 3674 3675 | N CA | ARG | | 83 | 31.994 | 2.522 | 94.830 | 1.00 38.75 |
| MOTA | 3676 | CB | ARG | | 83 | 31.865 | 3.616 | 95.885 | 1.00 40.24 1.00 49.12 |
| ATOM ATOM | 3677 | CG | ARG | | 83 | 33.187 | 4.180 | 96.330 97.404 | 1.00 49.12 |
| ATOM | 3678 | CD | ARG | | 83 | 33.015 34.240 | 5.239 6.010 | 97.624 | 1.00 59.30 |
| MOTA | 3679 | NE | ARG | | 83 83 | 35.437 | 5.486 | 97.883 | 1.00 61.56 |
| MOTA | 3680 | CZ | ARG ARG | | 83 | 35.598 | 4.170 | 97.958 | 1.00 63.53 |
| MOTA | 3681 3682 | NH1 | | | 83 | 36.479 | 6.285 | 98.073 | 1.00 62.02 |
| ATOM - MOTA | 3683 | C | ARG | | 83 | 32.719 | 1.326 | 95.426 | 1.00 37.75 1.00 37.18 |
| ATOM | 3684 | 0 | ARG | В | 83 | 33.893 | 1.094 | 95.146 96.249 | 1.00 37.10 |
| ATOM | 3685 | N | GLU | | 84 | 32.011 32.581 | 0.564 -0.609 | 96.898 | 1.00 35.29 |
| MOTA | 3686 | CA | GLU | | 84 84 - | 31.876 | -0.855 | 98.236 | 1.00 40.14 |
| MOTA | 3687 | CB CG | GLU GLU | | 84 | 30.443 | -0.383 | 98.240 | 1.00 46.30 |
| MOTA | 3688 3689 | CD | GLU | | 84 | 30.356 | 1.132 | 98.293 | 1.00 48.30 1.00 43.07 |
| ATOM ATOM | 3690 | OE1 | | | 84 | 29.339 | 1.690 | 97.834 | 1.00 43.07 |
| ATOM | 3691 | OE2 | GLU | | 84 | 31.306 | 1.762 -1.880 | 98.814 96.055 | 1.00 32.90 |
| ATOM | 3692 | C | GLU | | 84 | 32.527 33.371 | -2.765 | 96.193 | 1.00 28.68 |
| ATOM | 3693 | 0 | GLU LYS | | 84 85 | 31.533 | -1.984 | 95.187 | 1.00 27.12 |
| ATOM | 3694 3695 | N CA | LYS | | 85 | 31.412 | -3.177 | 94.361 | 1.00 30.46 |
| ATOM ATOM | 3696 | . CB | LYS | | 85 | 29.950 | -3.401 | 93.967 | 1.00 30.01 1.00 28.40 |
| ATOM | 3697 | CG | LYS | | 85 | 29.717 | -4.643 -4.807 | 93.117 92.775 | 1.00 32.87 |
| MOTA | 3698 | CD | LYS | | 85 | 28.234 28.000 | -6.048 | 91.928 | 1.00 34.15 |
| MC A | 3699 | CE | LYS | | 85 85 | 26.582 | -6.186 | 91.507 | 1.00 35.34 |
| A.OM | 3700 | NZ C | LYS | | 85 | 32.267 | -3.096 | 93.101 | 1.00 28.98 |
| MC_A MOTA | 3701 3702 | 0 | LYS | | 85 | 32.817 | -4.098 | | 1.00 24.69 1.00 27.81 |
| MOTA | 3703 | N | TYF | | 86 | 32.391 | -1.896 | | |
| ATOM | 3704 | | TY | | | 33.141 32.206 | -1.692 -1.050 | | |
| ATOM | 3705 | | TY | | | 32.208 | -1.927 | | 1.00 31.29 |
| MOTA | 3706 | | TYI 1 TYI | | | 31.178 | -3.137 | | 1.00 26.99 |
| ATOM | 3707 3708 | | | | | 30.095 | -3.955 | 88.965 | |
| MOTA MOTA | 3709 | | | | | 29.713 | -1.553 | | |
| MOTA | 3710 | | 2 TY | R B | 86 | 28.611 | | | 4/ |
| MOTA | 3711 | | TY | R B | | 28.815 | | | |
| ATOM | 3712 | OH | | R B | | 27.747 34.422 | | | 1.00 24.64 |
| ATOM | 3713 | | | R B R B | | 35.160 | _ | 90.530 | 1.00 27.19 |
| MOTA | 3714 | | | N E | | 34.674 | -0.41 | 92.71 | |
| ATOM | 3715 3716 | | | N E | - | 35.881 | 0.34 | 1 93.03 | |
| MOTA MOTA | 3717 | | AS | N E | 87 | 37.105 | | | |
| ATOM | | s co | : AS | N E | 3 87 | 38.343 | | | |
| ATOM | | 9 01 |)1 AS | N I | 87 | 38.309 | 0.43 | | - |
| | | | | | | | | | |

| | | MD2 | ASN B | 87 | 39.449 | 0.012 | 92.775 | 1.00 35.86 |
|-------|------|------|---------|------|--------|--------|--------|------------|
| MOTA | 3720 | | | | | | 92.223 | 1.00 29.72 |
| MOTA | 3721 | С | ASN B | 87 | 36.070 | | 91.876 | 1.00 24.01 |
| MOTA | 3722 | 0 | ASN B | 87 | 37.194 | | 91.070 | |
| | 3723 | N | ILE B | 88 | 34.956 | 2.282 | 91.932 | 1.00 29.43 |
| ATOM | | | ILE B | 88 | 34.945 | 3.536 | 91.196 | 1.00 30.64 |
| ATOM | 3724 | CA | | | 33.959 | 3.464 | 90.027 | 1.00 37.12 |
| ATOM- | 3725 | CB | ILE B | 88 | 33.939 | | | 1.00 40.62 |
| ATOM | 3726 | CG2 | ILE B | 88 | 33.821 | 4.829 | 89.379 | |
| | - | CG1 | ILE B | 88 | 34.421 | 2.433 | 89.008 | 1.00 35.43 |
| MOTA | 3727 | | | 88 | 35.684 | 2.821 | 88.324 | 1.00 41.80 |
| ATOM | 3728 | CD1 | | | | 4.669 | 92.118 | 1.00 31.90 |
| ATOM | 3729 | C | ILE B | 88 | 34.483 | | | 1.00 28.86 |
| ATOM | 3730 | 0 | ILE B | 88 | 33.681 | 4.445 | 93.024 | |
| | 3731 | N | GLY B. | 89 | 34.977 | 5.881 | 91.875 | 1.00 30.36 |
| ATOM | | | GLY B | 89 | 34.574 | 7.022 | 92.686 | 1.00 29.54 |
| ATOM | 3732 | CA | | | 35.601 | 7.524 | 93.685 | 1.00 31.49 |
| ATOM | 3733 | С | GLY B | 89 | | | 94.177 | 1.00 37.26 |
| MOTA | 3734 | 0 | GLY B | 89 | 35.497 | 8.652 | | 1.00 30.97 |
| MOTA | 3735 | N | GLY B | 90 | 36.583 | 6.687 | 94.005 | |
| | 3736 | CA | GLY B | 90 | 37.612 | 7.086 | 94.949 | 1.00 31.03 |
| MOTA | | | | 90 | 38.655 | 7.936 | 94.247 | 1.00 34.78 |
| MOTA | 3737 | С | GLY B | | 38.455 | 8.344 | 93.103 | 1.00 32.73 |
| MOTA | 3738 | 0 | GLY B | 90 | | | 94.915 | 1.00 29.39 |
| ATOM | 3739 | N | TYR B | 91 | 39.772 | 8.201 | | |
| | 3740 | CA | TYR B | 91 | 40.820 | 9.023 | 94.322 | 1.00 28.15 |
| MOTA | | | TYR B | 91 | 41.810 | 9.463 | 95.405 | 1.00 27.29 |
| MOTA | 3741 | CB | | | 42.609 | 8.330 | 96.007 | 1.00 26.60 |
| MOTA | 3742 | CG | TYR B | 91 | | 7.823 | 95.359 | 1.00 28.55 |
| MOTA | 3743 | CD1 | TYR B | 91 | 43.738 | | | 1.00 28.75 |
| ATOM | 3744 | CE1 | TYR B | 91 | 44.456 | 6.762 | 95.896 | |
| | 3745 | CD2 | | 91 | 42.219 | 7.741 | 97.208 | 1.00 28.35 |
| MOTA | _ | | | 91 | 42.927 | 6.680 | 97.751 | 1.00 27.58 |
| ATOM | 3746 | CE2 | | | 44.043 | 6.196 | 97.094 | 1.00 30.12 |
| MOTA | 3747 | CZ | TYR B | 91 | | | 97.637 | 1.00 36.59 |
| MOTA | 3748 | OH | TYR B | 91 | 44.753 | 5.154 | | 1.00 29.27 |
| MOTA | 3749 | C | TYR B | 91 | 41.563 | 8.271 | 93.226 | |
| | 3750 | ŏ | TYR B | 91 | 42.109 | 8.874 | 92.308 | 1.00 25.22 |
| MOTA | - | | | 92 | 41.568 | 6.948 | 93.318 | 1.00 28.32 |
| ATCM | 3751 | N | GLU B | | | 6.124 | 92.350 | 1.00 27.06 |
| ATOM | 3752 | CA | GLU B | 92 | 42.286 | | 92.924 | 1.00 23.35 |
| ATOM | 3753 | CB | GLU B | 92 | 42.474 | 4.726 | | 1.00 29.80 |
| | 3754 | CG | GLU B | 92 | 43.502 | 3.884 | 92.221 | 1.00 25.00 |
| MOTA | 3755 | CD | GLU B | 92 | 43.585 | 2.500 | 92.826 | 1.00 35.34 |
| MOTA | - | | | 92 | 42.742 | 1.645 | 92.477 | 1.00 32.15 |
| ATOM | 3756 | OE1 | | | | 2.278 | 93.678 | 1.00 31.61 |
| MOTA | 3757 | OE2 | | 92 | 44.475 | | 90.997 | 1.00 23.42 |
| ATOM | 3758 | C | GLU B | 92 | 41.594 | 6.024 | | 1.00 20.47 |
| | 3759 | 0 | GLU B | 92 | 42.204 | 6.260 | 89.962 | |
| MOTA | - | N | ASN B | 93 | 40.314 | 5.677 | 91.017 | 1.00 18.85 |
| MOTA | 3760 | | | 93 | 39.534 | 5.509 | 89.795 | 1.00 21.96 |
| ATOM | 3761 | CA | | | 39.165 | 4.033 | 89.664 | 1.00 23.90 |
| ATOM | 3762 | СB | ASN B | 93 | | 3.120 | 89.943 | 1.00 24.78 |
| ATCM | 3763 | CG | ASN B | 93 | 40.351 | _ | | 1.00 22.35 |
| ATOM | 3764 | ao c | l asn b | 93 | 41.362 | 3.160 | 89.239 | 1.00 22.35 |
| | 3765 | | 2 ASN B | 93 | 40.240 | 2.311 | 90.987 | 1.00 13.35 |
| ATOM | | | ASN B | 93 | 38.285 | 6.362 | 89.944 | 1.00 25.16 |
| ATOM | 3766 | C | | | 37.183 | 5.843 | 90.121 | 1.00 20.91 |
| ATOM | 3767 | 0 | ASN B | 93 | | 7.693 | 89.887 | 1.00 26.37 |
| ATCM | 3768 | N | PRO B | 94 | 38.449 | | | 1.00 19.35 |
| ATOM | 3769 | CD | PRO B | 94 | 39.738 | 8.389 | 89.716 | 1.00 13.55 |
| | 3770 | CA | PRO B | 94 | 37.373 | 8.676 | 90.024 | 1.00 24.59 |
| ATOM | _ | | | 94 | 38.147 | 9.972 | 90.200 | 1.00 25.95 |
| MOTA | 3771 | CB | PRO B | | 39.297 | 9.740 | 89.223 | 1.00 22.60 |
| MOTA | 3772 | ÇG | PRO B | 94 | | | 88.873 | 1.00 28.74 |
| ATOM | 3773 | C | PRO B | 94 | 36.384 | 8.777 | | 1.00 25.77 |
| | 3774 | 0 | PRO B | 94 | 36.562 | 8.176 | 87.808 | 1.00 23.77 |
| ATOM | | | VAL B | | 35.332 | 9.553 | 89.112 | 1.00 27.14 |
| MOTA | 3775 | N | | | 34.317 | 9.812 | 88.103 | 1.00 25.94 |
| MOTA | 3776 | CA | | | 34.31/ | 10.393 | 88.742 | 1.00 23.75 |
| ATOM | 3777 | CB | VAL B | 95 | 33.035 | | | 1.00 26.34 |
| | 3778 | CG | | | 32.067 | 10.855 | 87.662 | 1.00 20.54 |
| ATOM | | CG | | | 32.378 | 9.346 | 89.622 | 1.00 27.59 |
| atom | 3779 | | | | 34.912 | 10.861 | 87.175 | 1.00 25.69 |
| ATOM | 3780 | | VAL B | | | 11.793 | 87,641 | 1.00 25.25 |
| ATOM | 3781 | 0 | VAL B | | 35.564 | | 85.871 | |
| ATOM | 3782 | | SER B | | 34.708 | 10.699 | | |
| | 3783 | | _ | | 35.199 | 11.647 | 84.868 | |
| ATOM | | | - | | 36.729 | 11.705 | 84.850 | 03 00 |
| ATOM | 3784 | | | | 37.274 | 10.548 | 84.229 | 1.00 23.99 |
| > ∞OM | 3785 | OG | , ber c | , ,, | J | | | • |

| | 2706 | _ | SER B | 96 | 34.726 | 11.127 | | 1.00 26.22 |
|---------------|--------------|---------|--------|----------------|------------------|------------------|------------------|--------------------------|
| ATOM | 3786 3787 | С 0 | SER B | 96 | 33.943 | 10.174 | | 1.00 23.57 |
| ATOM | 3788 | N | TYR B | 97 | 35.195 | 11.744 | 02 | 1.00 22.83 |
| MOTA MOTA | 3789 | CA | TYR B | 97 | 34.818 | 11.279 | | 1.00 28.59 |
| MOTA | 3790 | СВ | TYR B | 97 | 34.536 | 12.452 | | 1.00 31.45 1.00 35.09 |
| ATOM | 3791 | CG | TYR B | 97 | 33.279 | 13.203 | 80.548 | 1.00 33.09 |
| ATOM | 3792 | CD1 | TYR B | 97 | 33.316 | 14.239 | 81.480 | 1.00 37.73 |
| MOTA | 3793 | CE1 | TYR B | 97 | 32.148 | 14.863 | 81.911 80.049 | 1.00 37.75 |
| ATOM | 3794 | CD2 | TYR B | | 32.036 | 12.812 | 80.475 | 1.00 38.61 |
| ATOM | 3795 | CE2 | TYR B | | 30.858 | 13.430 14.453 | 81.408 | 1.00 39.45 |
| ATOM | 3796 | CZ | TYR B | | 30.924 29.768 | 15.047 | 81.852 | 1.00 35.36 |
| MOTA | 3797 | OH | TYR B | | 35.883 | 10.354 | 80.534 | 1.00 28.93 |
| MOTA | 3798 | C | TYR B | | 35.859 | 9.992 | 79.358 | 1.00 28.26 |
| MOTA | 3799 | 0 | TYR E | | 36.822 | .9.968 | 81.385 | 1.00 29.09 |
| MOTA | 3800 3801 | N CA | ALA E | | 37.866 | 9.044 | 80.980 | 1.00 26.88 |
| MOTA | 3802 | CB | ALA E | | 39.167 | 9.369 | 81.692 | 1.00 27.99 |
| ATOM ATOM | 3803 | C | ALA E | | 37.395 | 7.657 | 81.382 | 1.00 22.53 1.00 21.98 |
| ATOM | 3804 | ŏ | ALA E | | 37.721 | 6.675 | 80.722 | 1.00 21.58 |
| ATOM | 3805 | N | MET E | 99 | 36.603 | 7.595 | 82.453 82.986 | 1.00 26.36 |
| MOTA | 3806 | CA | MET F | | 36.106 | 6.326 6.568 | 84.185 | 1.00 24.05 |
| ATOM | 3807 | CB | MET I | 3 99 | 35.179 33.822 | 7.188 | 83.875 | 1.00 28.37 |
| MOTA | 3808 | CG | MET I | | 33.822 | 7.704 | 85.406 | 1.00 27.91 |
| ATOM | 3809 | SD | MET I | | 33.106 | 6.227 | 86.409 | 1.00 22.12 |
| MOTA | 3810 | CE | MET I | | 35.430 | 5.435 | 81.953 | 1.00 25.76 |
| MOTA | 3811 | C | MET I | - ' | 35.544 | 4.212 | 82.031 | 1.00 26.11 |
| ATOM | 3812 3813 | O N | PHE | | 34.724 | 6.027 | 80.992 | 1.00 22.17 |
| MOTA | 3814 | CA | PHE | | 34.107 | 5.222 | 79.940 | 1.00 22.35 |
| MOTA MOTA | 3815 | CB | PHE | | 32.582 | 5.133 | 80.088 | 1.00 22.01 1.00 24.22 |
| MOTA | 3816 | CG | PHE : | | 31.947 | 4.254 | 79.038 | 1.00 24.22 |
| ATOM | 3817 | CDI | | | 32.143 | 2.872 | 79.061 77.953 | 1.00 21.22 |
| ATOM | 3818 | CD2 | PHE | | 31.280 | 4.813 2.059 | 78.012 | 1.00 26.91 |
| ATOM | 3819 | CE: | PHE | В 100 | 31.691 30.825 | 4.010 | 76.894 | 1.00 24.80 |
| MOTA | 3820 | CE2 | PHE | B 100 | 31.033 | 2.632 | 76.924 | 1.00 24.85 |
| MOTA | 3821 | CZ | PHE | B 100 B 100 | 34.425 | 5.695 | 78.514 | 1.00 24.86 |
| MOTA | 3822 | C | PHE | B 100 | 34.922 | 4.920 | 77.694 | 1.00 21.40 |
| MOTA | 3823 3824 | N O | THR | | 34.131 | 6.957 | 78.204 | 1.00 24.24 |
| MOTA | 3825 | CA | THR | | 34.390 | 7.469 | 76.854 | 1.00 24.54 1.00 24.46 |
| MOTA MOTA | 3326 | CB | THR | B 101 | 33.914 | 8.926 | 76.708 | 1.00 24.46 1.00 27.64 |
| ATOM | 3827 | OG | 1 THR | | 32.504 | | 76.953 75.297 | 1.00 27.04 |
| MOTA | 3828 | CG | 2 THR | B 101 | 34.191 | | 76.483 | 1.00 25.26 |
| ATOM | 3829 | C | THR | B 101 | 35.872 | | 75.430 | 1.00 25.47 |
| MOTA | 3830 | 0 | | B 101 | 36.231 36.725 | | | 1.00 23.74 |
| MOTA | 3831 | | | B 102 B 102 | 38.153 | | 77.096 | 1.00 24.53 |
| ATOM | 3832 | CA | CIV | B 102 | 38.657 | | 77.046 | 1.00 24.06 |
| ATOM | 3833 | | GLY | B 102 | 39.346 | | 76.100 | 1.00 22.53 |
| MOTA | 3834 3835 | | SER | B 103 | 38.316 | 5.651 | | 1.00 22.02 |
| MOTA | 3836 | | | B 103 | 38.730 | | | 1.00 20.45 1.00 25.21 |
| ATOM ATOM | 3837 | | SER | B 103 | 38.193 | | | 1.00 25.21 |
| ATOM | 3838 | | SER | в 103 | 38.820 | | | 1.00 20.53 |
| MOTA | 3839 | | SER | B 103 | 38.268 | | | 1.00 16.82 |
| ATOM | 3840 | _ | SER | B 103 | 39.034 | · | | |
| ATOM | 3841 | . N | SER | B 104 | 37.014 | | | 1.00 23.32 |
| MOTA | 3842 | | | B 104 | 36.462 34.980 | | | 1.00 22.93 |
| ATOM | 3843 | | SER | B 104 | 34.424 | | | 1.00 24.75 |
| MOTA | 3844 | | SER | B 104 B 104 | 37.22 | | 3 74.116 | 1.00 21.97 |
| MOTA | 3845 | | SEK | B 104 | 37.45 | _ | 73.256 | |
| ATOM | 3546 | | 35K | B 105 | 37.619 | 9 4.549 | 73.997 | |
| MOTA | 384 | | | B 105 | 38.35 | 4 5.00° | | |
| ATOM | 3848 3848 | | LEU | B 105 | 38.44 | | | |
| MOTA MOTA. | _ | 0 0 | LEU | B 105 | 38.70 | | | |
| MOTA. | - | | ol LEU | B 105 | 37.66 | 2 6.88 | 5 /0.312 | , <u>,</u> ,,,, |
| ALON | | | | | | | | |

| | | | - mrs D 105 | | 38.529 | 8.802 | 71.819 | 1.00 34.30 |
|------|--------|-----|------------------------|----|--------|--------|---|---|
| MOTA | 3852 | | LEU B 105 | | 39.755 | | 72.813 | 1.00 27.39 |
| MOTA | 3853 | С | LEU B 105 | | 40.262 | | 71.765 | 1.00 20.15 |
| ATOM | 3854 | 0 | LEU B 105 | | | 4.293 | 73.988 | 1.00 23.62 |
| MOTA | 3855 | N | ALA B 106 | | 40.371 | | 74.115 | 1.00 22.73 |
| ATOM | 3856 | CA | ALA B 106 | | 41.704 | 3.692 | | 1.00 17.46 |
| ATOM | 3857 | CB | ALA B 106 | | 42.263 | 3.939 | 75.529 | 1.00 22.77 |
| MOTA | 3858 | С | ALA B 106 | | 41.639 | 2.189 | 73.846 | |
| | 3859 | ō | ALA B 106 | | 42.583 | 1.597 | 73.316 | 1.00 24.98 |
| MOTA | 3860 | N | THR B 107 | | 40.523 | 1.567 | 74.224 | 1.00 23.54 |
| ATOM | 3861 | CA | THR B 107 | | 40.355 | 0.132 | 74.033 | 1.00 19.76 |
| ATOM | | CB | THR B 107 | | 39.236 | -0.410 | 74.947 | 1.00 22.85 |
| MOTA | 3862 | | THR B 107 | | 39.572 | -0.128 | 76.306 | 1.00 16.29 |
| ATOM | 3863 | OG1 | | | 39.085 | -1.917 | 74.787 | 1.00 17.21 |
| MOTA | 3864 | CG2 | THR B 107 | | 40.036 | -0.169 | 72.571 | 1.00 23.47 |
| MOTA | 3865 | C | _ | | 40.540 | -1.138 | 72.001 | 1.00 19.25 |
| MOTA | 3866 | 0 | THR B 107 GLY B 108 | | 39.191 | 0.656 | 71.959 | 1.00 24.87 |
| MOTA | 3867 | N | GLY B 100 | | 38.879 | 0.434 | 70.560 | 1.00 21.32 |
| MOTA | 3868 | CA | GLY B 108 | | 40.161 | 0.594 | 69.757 | 1.00 22.01 |
| ATOM | 3869 | C | GLY B 108 | | 40.388 | -0.099 | 68.761 | 1.00 20.46 |
| ATOM | 3870 | 0 | GLY B 108 | | 41.018 | 1.508 | 70.197 | 1.00 19.89 |
| ATOM | 3871 | Ŋ | SER B 109 | | 42.274 | 1.749 | 69.499 | 1.00 19.37 |
| ATOM | 3872 | CA | SER B 109 | | | 2.956 | 70.107 | 1.00 18.28 |
| MOTA | 3873 | CB | SER B 109 | | 42.993 | 4.145 | 69.882 | 1.00 21.29 |
| MOTA | 3874 | OG | SER B 109 | | 42.250 | 0.513 | 69.542 | 1.00 20.70 |
| ATOM | 3875 | С | SER B 109 | | 43.168 | | 68.617 | 1.00 20.69 |
| MOTA | 3876 | 0 | SER B 109 | | 43.940 | 0.261 | 70.616 | 1.00 20.54 |
| ATOM | 3877 | N | THR B 110 | | 43.065 | -0.259 | 70.729 | 1.00 19.98 |
| ATOM | 3878 | CA | THR B 110 | | 43.858 | -1.475 | 72.158 | 1.00 20.53 |
| ATOM | 3879 | CB | THR B 110 | | 43.826 | -2.043 | 73.007 | 1.00 20.72 |
| MOTA | 3880 | OG1 | THR B 110 | | 44.632 | -1.215 | _ | 1.00 20.05 |
| ATOM | 3881 | CG2 | THR B 110 | | 44.371 | -3.470 | 72.188 | 1.00 20.33 |
| ATOM | 3882 | C | THR B 110 | | 43.333 | -2.507 | 69.738 | 1.00 21.01 |
| MOTA | 3883 | Ō | THR B 110 | | 44.115 | -3.239 | 69.127 | 1.00 18.29 |
| ATOM | 3884 | N | VAL B 111 | | 42.012 | -2.557 | 69.567 | 1.00 20.36 |
| ATOM | 3885 | CA | VAL B 111 | | 41.432 | -3:486 | 68.608 | 1.00 23.94 |
| ATOM | 3886 | СВ | VAL B 111 | | 39.886 | -3.494 | 68.677 | 1.00 23.34 |
| | 3887 | CG | 1 VAL B 111 | | 39.324 | -4.442 | 67.619 | 1.00 21.50 |
| ATOM | 3888 | CG | | | 39.426 | -3.937 | 70.063 | |
| MOTA | 3889 | c c | VAL B 111 | | 41.872 | -3.080 | 67.197 | 1.00 20.35 |
| MOTA | 3890 | ō | VAL B 111 | | 42.146 | -3.936 | 66.362 | 1.00 23.29 |
| MOTA | | Ņ | GLN B 112 | ! | 41.953 | -1.775 | 66.937 | 1.00 22.07 |
| ATOM | 3892 | CA | GLN B 112 | | 42.367 | -1.290 | 65.617 | 1.00 22.34 |
| MOTA | 3893 | C3 | GLN B 112 | | 42.199 | 0.230 | 65.513 | 1.00 24.54 |
| MOTA | 3894 | CG | GLN B 112 | 2 | 40.810 | 0.729 | 65.843 | 1.00 20.63 |
| MOTA | 3895 | כם | | | 40.700 | 2.236 | 65.742 | 1.00 21.19 |
| MOTA | 3896 | OE | | | 40.664 | 2.794 | 64.645 | 1.00 26.73 |
| MOTA | | NE | 2 GLN B 112 | | 40.667 | 2.905 | 66.886 | 1.00 18.33 |
| ATOM | 3897 | C | GLN B 112 | 2 | 43.826 | -1.635 | 65.363 | 1.00 23. 1 |
| ATOM | 3898 | 0 | GLN B 11 | | 44.195 | -2.020 | 64.257 | 1.00 15.79 |
| ATOM | 3899 | N | ALA B 11 | 3 | 44.660 | -1.476 | 66.389 | 1.00 20.60 |
| MOTA | 3900 | | | 3 | 46.070 | -1.790 | 66.249 | 1.00 18.02 |
| ATOM | 3901 | | | ž. | 46.794 | -1.536 | 67.548 | 1.00 20.84 |
| MOTA | 3902 | | ALA B 11 | á | 46.170 | | 65.863 | 1.00 23.78 |
| MOTA | 3903 | | ALA B 11 | | 46.982 | -3.642 | 65.023 | 1.00 19.33 |
| MOTA | 3904 | | ILE B 11 | | 45.331 | | | 1.00 21.45 |
| ATOM | . 3905 | | | | 45.344 | | | 1.00 24.26 |
| ATOM | 3906 | | ILE B 11 | 4 | 44.507 | | | 1.00 20.72 |
| MOTA | 3907 | | | 4 | 44.476 | | | 1.00 21.92 |
| MOTA | 3908 | | | 4 | | | | 1.00 24.32 |
| ATOM | 3909 | | 1 ILE B 11 | 4 | 45.116 | | | 1.00 19.01 |
| ATOM | 3910 | | 1 ILE B 11 | 4 | 44.364 | | | 1.00 26.75 |
| ATOM | 3911 | | ILE B 11 | 4 | 44.808 | -6.640 | | 1.00 20.18 |
| ATOM | 3912 | | ILE B 11 | 4 | 45.305 | | | 1.00 24.59 |
| ATOM | 3913 | | GLU B 11 | 5 | 43.792 | | | 1.00 29.26 |
| MOTA | | | GLU B 11 | 5 | 43.243 | -5.198 | | |
| ATOM | | | GLU B 11 | 5 | 42.043 | | | |
| ATOM | 4 / | | GLU B 11 | 5 | 40.940 | | | 14 |
| ATOM | | | 11 | .5 | 39.757 | -3.519 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| ATOM | | | | | | | | |

| | | | • | | | 6 | | | | | | | | | |
|---|---|---|---|---------------------------------------|--|--|--|--|---|--|---|--|--|--------------------------------------|----------------------------|
| AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA | TOM | 89190123456789012345678992223456789933933939333333333333333333333333333 | C O N CAB G O C C C C C C O N CAB G D D C C C C C C O N CAB G D D C C C C C C C C C C C C C C C C C | B B B B B B B B B B B B B B B B B B B | 11111111111111111111111111111111111111 | 334445.290.543.28445.290.543.28445.290.543.28445.290.543.28445.290.543.28445.290.543.284445.290.543.284445.290.543.284445.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.2844444.290.543.284444.290.543.284444.290.543.284444.290.543.284444.290.543.284444.290.543.28444.290.543.28444.290.543.28444.290.543.28444.290.543.28444.290.543.28444.290.543.28444.290.543.28444.290.543.290.290.290.290.290.290.290.290.290.290 | 0344169565721686466449920133327087491556486702982872982133327087492417356486702982855857087491498285 | -8. -9. -7. -6. -5. -3. -2. -1. -6. -7. -5. -3. -2. -1. -5. -2. -2. -2. -2. -2. -2. -3. -2. -3. -3. -3. -3. -3. -3. -3. -3 | 406 039 227 837 44 44 45 79 21 21 21 21 21 21 22 22 29 73 74 14 44 45 77 25 21 21 21 21 22 26 27 27 27 28 28 28 28 28 28 28 28 28 28 28 28 28 | 57. 57. 58. 58. 58. 57. | 884444451133535448930059344026691509978866247738842198584409958691509978866884119888410995869173350 | 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 | 391. 32266. 3326 | 854341122355882377533473795087259025 | 15312)51694133525581529754 |
| | MOTA | 3962 | 0 | GLY | B 120 | | | | | 58. | 600 | 1.0 | 0 2 | 5.4 | 2 |
| | | | | ASN | в.21 | 50. | 695 | -3 | . 587 | 58. | 919 | 1.0 | 0 2 0 3 | 9.4 | 9 |
| | ATCM | 3965 | CB | ASN | B 121 | | | -2 | .307 | 57. | 325 | 1.0 | 0 3 | 2.2 | :5 |
| | ATOM ATOM | 3967 | | ASN | B 121 | 49 | .924 | -2 | | | 350 217 | | 0 3 | $\frac{5.4}{2.2}$ | 26 |
| | ATOM | 3968 | ND2 | ASN | B 121 | | .917 .172 | | .006 | 60. | 361 | 1.0 | 0 3 | 0.9 | 2 |
| | ATOM | 3969 3970 | | ASN | B 121 B 121 | | .971 | -4 | .631 | 61. | . 059 | | 0 2 | 7.0 | 8 |
| | MOTA MOTA | 3971 | | VAL | B 122 | | .810 | | .560 | | .796 .155 | | 00 2 | 29.4 | 18 |
| | ATOM | 3972 | CA | VAL | B 122 | | .309 .840 | | .457 .352 | | . 177 | 1.0 | 0 3 | 33.4 | 10 |
| | MOTA | 3973 | | VAL. | B 122 B 122 | | .334 | | .294 | 63 | .611 | 1.0 | 00 3 | 32.2 | 22 |
| | MOTA MOTA | 3974 3975 | - | VAL | B 122 | | .446 | | .544 | | .458 .748 | | 00 2 | 33.! 29.(| 04 |
| | ATOM | 397 | 5 C | VAL | B 122 | | .713 | | .196 .118 | | .153 | 1.0 | 00 2 | 27. | 4.7 |
| | ATOM | 397 | | VAL 21.2 | B 122 B 123 | | .100 |) -1 | 326 | 63 | .918 | 1. | 00 3 | 26.° 25. | 71 |
| | ATOM ATOM | 397: 397 | | ALA | B 123 | 50 | .47 | 7 -0 | 177 | | .559 | | 00 | 25. 21. | 65 |
| | ATOM | 398 | 0 CB | ALA | в 123 | 48 50 | .96 .87 | 2 -0 2 -0 |).281).005 | | .017 | 1 1. | 00 | 28. | 62 |
| | ATOM | 398 | | الملك حراج | В 123 В 123 | 51 | . 22 | 7 -0 | .965 | 66 | .712 | 2 1. | | 26. 22. | |
| | ATOM ATOM | 200 | _ | PHE | B 124 | | .80 | | 1.239 | 66 | .472 | ٤ 1. | 00 | ~~. | 0 3 |
| | | | | | | | | | | | | | | | |

| | | CA PHE B 124 | 51.122 | 1.577 | | 1.00 17.31 |
|-------|------|-----------------|--------|--------|--------|------------|
| ATOM | 3984 | | 52.419 | | 67.876 | 1.00 16.88 |
| ATOM | 3985 | CB PHE B 124 | 32.413 | | | 1.00 18.52 |
| ATOM | 3986 | CG PHE B 124 | 52.762 | | | 1.00 17.52 |
| | 3987 | CD1 PHE B 124 | 52.533 | | . • | |
| MOTA | | CD2 PHE B 124 | 53.382 | 4.245 | | 1.00 17.88 |
| MOTA | 3988 | | 52.914 | 2.837 | 71.638 | 1.00 25.77 |
| ATOM- | 3989 | | 53.769 | | | 1.00 21.97 |
| MOTA | 3990 | CE2 PHE B 124 | | | 71.698 | 1.00 20.16 |
| MOTA | 3991 | CZ PHE B 124 | 53.535 | | | 1.00 18.77 |
| | 3992 | C PHE B 124 | 49.937 | 2.348 | 68.421 | |
| ĄTOM | | 101 | 49.462 | 3.311 | 67.820 | 1.00 16.62 |
| ATOM | 3993 | | 49.418 | 1.868 | 69.546 | 1.00 16.69 |
| ATOM | 3994 | | | | 70.238 | 1.00 16.22 |
| MOTA | 3995 | CA ASN B 125 | 48.320 | | 70.435 | 1.00 12.71 |
| ATOM | 3996 | CB ASN B 125 | 47.129 | | | 1.00 19.79 |
| | 3997 | CG ASN B 125 | 46.095 | 2.209 | 71.346 | |
| ATOM | | OD1 ASN B 125 | 45.930 | 3.430 | 71.372 | 1.00 20.83 |
| ATOM | 3998 | | 45.376 | 1.371 | 72.087 | 1.00 12.31 |
| MOTA | 3999 | | 48.790 | 3.004 | 71.600 | 1.00 19.19 |
| MOTA | 4000 | C ASN B 125 | | 2.280 | 72.585 | 1.00 20.99 |
| MOTA | 4001 | O ASN B 125 | 48.687 | | 71.668 | 1.00 19.02 |
| ATOM | 4002 | N PRO B 126 | 49.335 | 4.226 | | 1.00 21.39 |
| | 4003 | CD PRO B 126 | 49.595 | 5.156 | 70.555 | |
| MOTA | 4004 | CA PRO B 126 | 49.833 | 4.805 | 72.917 | 1.00 21.60 |
| ATOM | | 106 | 50.398 | 6.161 | 72.459 | 1.00 21.07 |
| MOTA | 4005 | CB PRO B 126 | 49.530 | 6.487 | 71.269 | 1.00 17.70 |
| MOTA | 4006 | CG PRO B 126 | | 4.942 | 74.034 | 1.00 20.69 |
| ATOM | 4007 | C PRO B 126 | 48.808 | | 75.198 | 1.00 19.79 |
| ATOM | 4008 | O PRO B 126 | 49.178 | 5.053 | | 1.00 16.67 |
| | 4009 | N ALA B 127 | 47.525 | 4.937 | 73.689 | |
| ATOM | | CA ALA B 127 | 46.476 | 5.065 | 74.698 | 1.00 20.44 |
| ATOM | 4010 | | 45.198 | 5.609 | 74.066 | 1.00 19.56 |
| ATOM | 4011 | | 46.169 | 3.747 | 75.401 | 1.00 20.80 |
| ATOM | 4012 | | 45.555 | 3.742 | 76.472 | 1.00 19.47 |
| MOTA | 4013 | O ALA B 127 | 46.587 | 2.634 | 74.800 | 1.00 20.52 |
| MOTA | 4014 | N GLY B 128 | | 1.333 | 75.399 | 1.00 19.43 |
| ATOM | 4015 | CA GLY B 128 | 46.325 | 0.910 | 76.463 | 1.00 20.56 |
| MOTA | 4016 | C GLY B 128 | 47.327 | | 76.869 | 1.00 18.37 |
| ATOM | 4017 | O GLY B 128 . | 48.182 | 1.697 | | 1.00 19.68 |
| ATOM | 4018 | N GLY B 129 | 47.215 | -0.333 | 76.929 | 1.00 19.93 |
| | 4019 | CA GLY B 129 | 48.136 | -0.820 | 77.943 | 1.00 15.35 |
| ATOM | 4020 | C GLY B 129 | 47.620 | -0.619 | 79.358 | 1.00 25.25 |
| ATOM | | 120 | 48.383 | -0.686 | 80.329 | 1.00 18.98 |
| ATOM | 4021 | | 46.317 | -0.374 | 79.474 | 1.00 16.04 |
| ATOM | 4022 | | 45.677 | -0.161 | 80.768 | 1.00 19.26 |
| ATOM | 4023 | | 44.301 | 0.451 | 80.519 | 1.00 17.94 |
| ATOM | 4024 | CB MET B 130 | | 1.728 | 79.653 | 1.00 22.95 |
| ATOM | 4025 | CG MET B 130 | 44.413 | | 79.307 | 1.00 31.83 |
| ATOM | 4026 | SD MET B 130 | 42.873 | 2.615 | 78.382 | 1.00 20.22 |
| | 4027 | CE MET B 130 | 41.957 | 1.358 | | 1.00 22.63 |
| ATOM | 4028 | C MET B 130 | 45.598 | -1.548 | 81.421 | 1.00 22.03 |
| ATOM | | O MET B 130 | 44.546 | -2.173 | 81.486 | 1.00 16.24 |
| ATOM | 4029 | | 46.737 | -1.999 | 81.932 | 1.00 18.42 |
| ATOM | 4030 | N HIS B 131 | 46.853 | -3.343 | 82.472 | 1.00 17.07 |
| ATOM | 4031 | CA HIS B 131 | 48.323 | -3.804 | 82.341 | 1.00 17.61 |
| ATOM | 4032 | CB HIS B 131 | 49.316 | -2.979 | 83.106 | 1.00 14.01 |
| ATOM | 4033 | CG HIS B 131 | | | 83.915 | 1.00 13.47 |
| ATOM | 4034 | CD2 HIS B 131 | 49.138 | -1.904 | | 1.00 18.00 |
| ATOM | 4035 | ND1 HIS B 131 | 50.680 | -3.190 | 83.051 | 1.00 15.27 |
| | 4036 | | 51.297 | -2.281 | 83.789 | 1.00 13.27 |
| ATOM | 4037 | | 50.384 | -1.489 | 84.324 | 1.00 17.21 |
| ATOM | | 431 | 46.329 | -3.724 | 83.852 | 1.00 16.41 |
| ATOM | 4038 | | 46.452 | -4.883 | 84.236 | 1.00 19.37 |
| ATOM | 4039 | | 45.721 | -2.794 | 84.586 | 1.00 18.64 |
| ATOM | 4040 | N HIS B 132 | | -3.112 | 85.936 | 1.00 20.87 |
| ATOM | 4041 | CA HIS B 132 | 45.241 | | | |
| ATOM | 4042 | CB HIS B 132 | 45.513 | -1.935 | | |
| | 1043 | 430 | 46.966 | -1.686 | | |
| ATOM | 1044 | | 47.715 | -0.563 | | |
| ATOM | | | 47.810 | -2.655 | 87.659 | |
| ATOM | 4045 | | 49.014 | -2.139 | 87.837 | |
| ATOM | 4046 | . AES ATC B 135 | 48.984 | -0.872 | | 1.00 14.88 |
| ATOM | 404 | 177 | 43.778 | -3.547 | | 1.00 22.83 |
| ATOM | 4048 | 177 | 43.478 | -4.298 | | |
| ATOM | | O HIS B 132 | 45.470 | -3,230 | | |
| | | | | | | |

| | | | | | | 2 000 | 85.271 | 1.00 16.54 |
|------|------|-----|-----------|----|--------|---------|----------|--------------------|
| MOTA | 4050 | N | ALA B 133 | | 42.878 | -3.088 | | 1.00 19.13 |
| ATOM | 4051 | CA | ALA B 133 | } | 41.457 | -3.396 | 85.424 | 1.00 23.56 |
| ATOM | 4052 | CB | ALA B 133 | } | 40.654 | -2.704 | 84.328 | 1.00 23.30 |
| | 4053 | C | ALA B 13 | | 41.127 | -4.883 | 85.439 | 1.00 23.12 |
| MOTA | | ō | ALA B 13 | | 41.718 | -5.677 | 84.696 | 1.00 18.03 |
| MOTA | 4054 | | PHE B 13 | | 40.181 | -5.257 | 86.294 | 1.00 19.69 |
| MOTA | 4055 | N | | | 39.762 | -6.649 | 86.365 | 1.00 19.35 |
| MOTA | 4056 | CA | PHE B 13 | | | | 87.818 | 1.00 21.26 |
| ATOM | 4057 | CB | PHE B 13 | | 39.583 | -7.122 | | 1.00 23.41 |
| ATOM | 4058 | CG | PHE B 13 | 1 | 40.837 | -7.053 | 88.646 | 1.00 23.41 |
| ATOM | 4059 | CD1 | PHE B 13 | 4 | 41.041 | -6.009 | 89.544 | 1.00 24.25 |
| | 4060 | CD2 | PHE B 13 | 4 | 41.820 | -8.027 | 88.522 | 1.00 22.80 |
| ATOM | 4061 | CE1 | | | 42.207 | -5.935 | 90.311 | 1.00 23.36 |
| MOTA | | CE2 | | | 42.997 | -7.964 | 89.283 | 1.00 27.74 |
| MOTA | 4062 | | PHE B 13 | | 43.190 | -6.917 | 90.178 | 1.00 24.05 |
| MOTA | 4063 | cz | | | 38.444 | -6.816 | 85.621 | 1.00 18.60 |
| MOTA | 4064 | C | PHE B 13 | | 37.815 | -5.849 | 85.196 | 1.00 13.82 |
| ATOM | 4065 | 0 | PHE B 13 | | | -8:.064 | 85.454 | 1.00 19.78 |
| ATOM | 4066 | N | LYS B 13 | | 38.050 | | 84.782 | 1.00 28.09 |
| ATOM | 4067 | CA | LYS B 13 | 5 | 36.813 | -8.421 | | 1.00 34.06 |
| ATOM | 4068 | CB | LYS B 13 | 5 | 36.501 | -9.879 | 85.125 | |
| ATOM | 4069 | CG | LYS B 13 | 5 | | -10.310 | 84.953 | 1.00 42.76 |
| | 4070 | CD | LYS B 13 | 5 | 34.927 | -11.745 | 85.437 | 1.00 48.44 |
| MOTA | 4071 | CE | LYS B 13 | 5 | 33.462 | -12.152 | 85.531 | 1.00 55.66 |
| MOTA | | NZ | LYS B 13 | | 32.727 | -11.332 | 86.544 | 1.00 51.65 |
| ATOM | 4072 | | LYS B 13 | | 35.639 | -7.512 | 85.172 | 1.00 28.27 |
| MOTĄ | 4073 | C | TIS D 13 | | 34.927 | -6.999 | 84.309 | 1.00 24.86 |
| MOTA | 4074 | 0 | LYS B 13 | | 35.450 | -7.292 | 86.470 | 1.00 29.89 |
| ATOM | 4075 | N | SER B 13 | | | -6.477 | 86.933 | 1.00 30.86 |
| ATOM | 4076 | CA | SER B 13 | | 34.331 | | 87.582 | 1.00 31.57 |
| MOTA | 4077 | CB | SER B 13 | | 33.282 | -7.388 | | 1.00 45.10 |
| ATOM | 4078 | OG | SER B 13 | | 32.916 | -8.434 | 86.698 | 1.00 31.50 |
| ATOM | 4079 | С | SER B 13 | | 34.705 | -5.380 | 87.923 | 1.00 31.50 |
| MOTA | 4080 | 0 | SER B 13 | 6 | 33.887 | -4.997 | 88.765 | 1.00 24.34 |
| ATOM | 4081 | N | ARG B 13 | | 35.920 | -4.854 | 87.835 | 1.00 22.63 |
| | 4082 | CA | ARG B 13 | | 36.291 | -3.826 | 88.794 | 1.00 25.51 |
| ATOM | | CB | ARG B 13 | | 36.629 | -4:486 | 90.136 | 1.00 29.62 |
| ATOM | 4083 | | ARG B 13 | 7 | 36.391 | -3.578 | 91.318 | 1.00 36.21 |
| MOTA | 4084 | CG | ARG B 13 | 7 | 36.874 | -4.160 | 92.631 | 1.00 40.79 |
| MOTA | 4085 | CD | ARG B 13 | 7 | 36.365 | -3.357 | 93.744 | 1.00 45.95 |
| MOTA | 4086 | NE | ARG B 13 | 7 | 36.863 | -3.369 | 94.973 | 1.00 41.97 |
| MOTA | 4087 | CZ | ARG B 13 | | 37.897 | -4.144 | 95.263 | 1.00 43.42 |
| ATOM | 4088 | NH. | ARG B 13 | 57 | | -2.604 | 95.913 | 1.00 46.65 |
| ATOM | 4089 | NH | | | 36.322 | -2.956 | 88.339 | 1.00 24.73 |
| ATOM | 4090 | С | ARG B 13 | | 37.461 | | 87.734 | 1.00 19.32 |
| ATOM | 4091 | 0 | ARG B 13 | | 38.420 | | | 1.00 16.77 |
| MOTA | 4092 | N | ALA B 1 | 38 | 37.372 | | 88.631 | 1.00 18.50 |
| ATOM | 4093 | CA | ALA B 1 | | 38.428 | | 88.270 | |
| ATOM | 4094 | СВ | ALA B 1 | 38 | 37.939 | | 88.401 | |
| | 4095 | C | ALA B 1 | | 39.597 | -0.964 | 89.216 | 1.00 22.62 |
| ATOM | 4096 | ō | ALA B 1 | | 39 411 | -1.419 | 90.346 | 1.00 18.98 |
| MOTA | 4097 | N | ASN B 1 | 39 | 40.301 | | 88.759 | 1.00 20.82 |
| MOTA | | | ASN B 1 | 19 | 41.989 | | 89.585 | 1.00 25.17 |
| ATOM | 4098 | CA | ASN B 1 | 30 | 42.311 | | 89.689 | 1.00 20.59 |
| ATOM | 4099 | CB | ASN B 1 | 20 | 43.556 | | 90.511 | 1.00 27.70 |
| MOTA | 4100 | CG | ASN B 1 | 22 | 43.726 | | 91.592 | 1.00 22.43 |
| ATOM | 4101 | αo | 1 ASN B 1 | 39 | | | 90.010 | 1.00 24.43 |
| ATOM | 4102 | ND | | | 44.420 | | 89.020 | |
| MOTA | 4103 | С | ASN B 1 | | 43.176 | | | |
| ATOM | 4104 | 0 | ASN B 1 | | 43.338 | | 87.799 | |
| ATOM | 4105 | N | GLY B 1 | 40 | 43.984 | | 89.920 | |
| | 4106 | | GLY B 1 | 40 | 45.166 | | 89.524 | |
| MOTA | 4107 | | GLY B 1 | 40 | 45.005 | | | |
| ATOM | 4107 | | GLY B 1 | | 45.827 | 7 2.301 | | 1.00 22.47 |
| ATOM | | | PHE B 1 | 41 | 43.958 | | 88.473 | 1.00 22.33 |
| MOTA | 4109 | | 1 | 41 | 43.694 | 4.126 | 87.461 | |
| ATOM | 4110 | | 1 | 41 | 44.996 | | 86.997 | |
| MOTA | 4111 | | PRE D 1 | 41 | 45.810 | | | 1.00 23.17 |
| ATOM | 4112 | CG | PHE B 1 | 41 | 47.11 | | | 1.00 22.17 |
| MOTA | 4113 | CI | 1 PHE B 1 | 41 | 45.28 | | | 1.00 23.40 |
| ATOM | 4114 | CI | 2 PHE B 1 | 41 | | | | |
| ATOM | 4115 | CE | 1 PHE B 1 | 41 | 47.87 | 0,402 | , 55,000 | · - - · |
| | | | | | | | | |

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|--------------|--------------|------------|-------|----------------|----|------------------|------------------|------------------|---------|----------------------|
| > moM | 4116 | CE2 | PHE B | 141 | | . 033 | 6.244 | 90.361 | | 23.03 |
| ATOM | 4117 | | PHE B | | 47 | . 335 | 6.658 | 90.092 | | 25.15 |
| ATOM ATOM | 4118 | | PHE B | | | .029 | 3.538 | 86.214 | | 23.69 18.88 |
| ATOM | 4119 | 0 | PHE B | 141 | | . 596 | 4.283 | 85.33 | | 15.03 |
| ATOM | 4120 | N | CYS B | 142 | | .962 | 2.211 | 86.127 | | 19.55 |
| ATOM | 4121 | CA | CYS B | 142 | | .380 | 1.578 | 84.93 | | 20.38 |
| ATOM | 4122 | CB | CYS B | 142 | | .193 | 0.336 | | | 37.40 |
| ATOM | 4123 | SG | CYS B | 142 | | .933 | 0.662 | | | 22.77 |
| MOTA | 4124 | С | CYS B | 142 | 40 | .923 | 1.171 | | | 23.04 |
| MOTA | 4125 | 0 | CYS B | 142 | | .561 | 0.514 | | | 15.24 |
| MOTA | 4126 | N | TYR B | 143 | | .094 | 1.194 | | | 21.97 |
| MOTA | 4127 | CA | TYR B | 143 | | .675 .795 | 2.372 | | | 18.06 |
| MOTA | 4128 | CB | TYR B | | | .016 | 3.622 | | 5 1.00 | 24.34 |
| ATOM | 4129 | CG | TYR B | 143 | | .038 | 4.516 | | 4 1.00 | 23.20 |
| MOTA | 4130 | CD1 | TYR B | 143 | | .265 | 5.658 | | 1 1.00 | 27.42 |
| MOTA | 4131 | CEI | TYR B | 143 | | .226 | 3.892 | 85.65 | 2 1.00 | 19.15 |
| MOTA | 4132 | CD2 CE2 | TYR B | 143 | | .441 | 5.023 | 86.43 | | 21.92 |
| ATOM | 4133 | CZ | TYR B | | 38 | .458 | 5.900 | 86.09 | | 23.94 |
| MOTA | 4134 4135 | OH | TYR B | | 38 | .655 | 7.015 | | | 22.37 |
| MOTA | 4136 | C | TYR B | | 38 | .431 | 0.008 | | | 19.91 22.50 |
| MOTA MOTA | 4137 | ō | TYR B | | | .665 | -0.902 | | | 19.20 |
| MOTA | 4138 | N | ILE B | 144 | | .083 | 0.026 | | | 19.68 |
| ATOM | 4139 | CA | ILE B | 144 | | .938 | -1.05 | | | 20.26 |
| ATOM | 4140 | CB | ILE B | 144 | | 3.282 | -0.528 -1.649 | | | |
| MOTA | 4141 | CG2 | ILE B | 144 | | 3.151 5.901 | 0.05 | | | 20.93 |
| ATOM | 4142 | CG1 | ILE B | 144 | | 5.198 | 0.69 | | | 23.75 |
| MOTA | 4143 | CD1 | ILE B | 144 | |).320 | -1.62 | | 74 1.00 | 22.78 |
| MOTA | 4144 | С | ILE B | 144 | | 1.281 | -0.87 | 3 80.60 | | 22.01 |
| MOTA | 4145 | 0 | ASN B | 145 | | .422 | -2.95 | 6 80.73 | | 23.18 |
| MOTA | 4146 4147 | N CA | ASN B | 145 | | 1.698 | -3.62 | 3 80.45 | | 20.63 |
| ATOM | 4148 | CB | ASN B | 145 | | 1.778 | -4.93 | | | 17.81 |
| ATOM ATOM | 4149 | CG | ASN B | | | 3.188 | -5.53 | | | 25.17 23.63 |
| ATOM | 4150 | OD1 | ASN B | 145 | | 3.804 | -5.74 | | | 22.69 |
| MOTA | 4151 | ND2 | ASN B | 145 | | 3.693 | -5.81 | - | | |
| MOTA | 4152 | С | ASN B | | | 1.780 | -3.91 -5.00 | | | |
| ATOM | 4153 | 0 | ASN E | | | 1.389 2.293 | -2.96 | | | 0 15.23 |
| MOTA | 4154 | N . | ASN E | | | 2.253 | -3.17 | | | |
| MOTA | 4155 | CA | ASN E | 146 | | 2.773 | -1.88 | | | |
| MOTA | 4156 | CB CG | ASN E | | _ | 4.196 | -1.45 | 8 76.3 | 06 1.0 | |
| ATOM | 4157 4158 | | ASN E | | | 5.109 | -1.73 | 5 75.5 | | 0 20.27 |
| MOTA | 4159 | ממא | ASN E | | 4 | 4.395 | -0.79 | | | 0 11.85 0 19.07 |
| ATOM | 4160 | C | ASN I | | 4 | 3.277 | -4.34 | | | 0 19.61 |
| MOTA MOTA | 4161 | ō | ASN I | 3 146 | | 3.030 | -4.99 | 6 75.3 8 77.0 | | 0 17.78 |
| MOTA | 4162 | N | PRO I | в 147 | | 4.358 | -4.59 | | | 0 18.13 |
| MOTA | 4163 | CD | PRO I | B 147 | | 4.953 | -3.91 -5.73 | | | 0 19.98 |
| ATOM | 4164 | CA | PRO I | В 147 | | 5.197 | -5.69 | | | 0 24.29 |
| MOTA | 4165 | CB | PRO I | B 147 | | 6.338 | -4.20 | | _ | 0 26.27 |
| ATOM | 4166 | CG | PRO | B 147 | | 4.377 | -7.0 | · | 757 1.0 | 0 20.91 |
| MOTA | 1167 | | PRO | B 147 | | 4.461 | -7.89 | | 371 1.0 | 0 17.58 |
| ATOM | 4168 | | PRO ! | B 147 B 148 | | 3.568 | -7.1 | | 309 1.0 | 0 15.81 |
| MOTA | 4169 | | ALM : | B 148 | | 2.732 | -8.3 | 62 78.0 | | 0 19.82 |
| MOTA | 4170 | | 21.2 | B 148 | | 2.049 | -8.3 | 12 79. | _ | 0 17.50 |
| MOTA | 4171 | | A.1.A | в 148 | | 1.683 | -8.4 | | | 0 22.58 |
| ATOM | 4172 | | ALA | B 148 | 4 | 1.419 | -9.5 | | | 00 18.38 00 22.48 |
| ATOM | 4174 | | VAL | в 149 | | 1.080 | | | | 0 19.04 |
| ATOM | 4175 | CA | VAL | B 149 | 4 | 10.086 | -7.3 | | 100 I.U | 00 18.96 |
| ATOM | 4176 | | VAL | B 149 | : | 9.503 | -5.8 | | | 00 17.32 |
| MOTA MOTA | 4177 | | 1 VAL | B 149 | | 38.691 | | | 462 1.0 | 00 15.33 |
| ATOM | 4178 | | 2 VAL | B 149 | | 38.621 | | ~ | 166 1.0 | 00 22.12 |
| ATOM | 4179 | | VAL | B 149 | | 40.763 40.240 | | | 421 1.0 | 00 21.83 |
| ATOM | 4180 | 0 | VAL | B 149 | • | 40.240 41.927 | -0.3 -7.1 | | | 00 19.51 |
| ATOM | 418 | 1 N | GLY | в 150 | ' | 2 L . J L / | .,.1 | | | |
| = | | | | | | | | | | |

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|---|--------------|--------------|------------|------------------------|-----|------------------|--------------------|------------------|--------------------------|
| | | | <i>c</i> > | GLY B 150 | | 42.657 | -7.433 | | 1.00 19.32 |
| | MOTA | 4182 | CA | GLY 3 150 | | 43.033 | -8.901 | | 1.00 19.59 |
| | MOTA | 4183 | C | GLY B 150 | | 42.862 | -9.550 | 71.568 | 1.00 22.28 |
| | MOTA | 4184 | O N | ILE B 151 | | 43.558 | -9.435 | 73.700 | 1.00 19.51 |
| | MOTA | 4185 | N CA | ILE B 151 | | 43.958 - | -10.834 | 73.723 | 1.00 23.21 |
| - | MOTA | 4186 | CE | ILE B 151 | | 44.666 - | -11.175 | 75.053 | 1.00 23.50 |
| | MOTA | 4187 | CG2 | ILE B 151 | | 44.918 - | -12.679 | 75.158 | 1.00 20.01 |
| | MOTA | 4188 | CG1 | ILE B 151 | | 45.988 - | -10.394 | 75.129 | 1.00 21.98 |
| | MOTA | 4189 | | ILE B 151 | | 46.716 - | -10.502 | 76.457 | 1.00 21.24 |
| | MOTA | 4190 4191 | CDI | ILE B 151 | | 42.749 | -11.741 | 73.490 | 1.00 28.40 |
| | MOTA | 4192 | 0 | ILE B 151 - | | 42.832 | -12.692 | 72.706 | 1.00 22.96 |
| | MOTA | 4193 | N | GLU B 152 | | 41.623 | -11.450 | 74.144 | 1.00 27.32 |
| | MOTA | 4194 | CA | GLU B 152 | | 40.417 | -12.265 | 73.939 | 1.00 27.62 |
| | ATOM | 4195 | СВ | GLU B 152 | | 39.294 | -11.845 | 74.886 | 1.00 26.46 |
| | MOTA | 4196 | CG | GLU B 152 | | 39.533 | -12.200 | 76.347 | 1.00 28.26 |
| | MOTA | 4197 | CD | GLU B 152 | | 39.513 | -13.708 | 76.592 | 1.00 31.10 |
| | ATOM ATOM | 4198 | OE1 | | | 39.668 | -14.123 | 77.767 | 1.00 29.55 1.00 30.51 |
| | | 4199 | OE2 | GLU B 152 | | 39.626 | -14.481 | 75.617 | 1.00 30.31 |
| | ATOM ATOM | 1200 | C | GLU B 152 | | 39.948 | -12.125 | 72.497 | 1.00 25.58 |
| | ATOM | 4201 | ō | GLU B 152 | | 39.463 | -13.082 | 71.893 | 1.00 26.23 |
| | ATOM | 4202 | N | TYR B 153 | | | -10.923 | 71.948 70.563 | 1.00 28.19 |
| | ATOM | 4203 | CA | TYR B 153 | | 39.720 | | 70.303 | 1.00 27.94 |
| | ATOM | 4204 | CB | TYR B 153 | | 40.082 | -9.235 | 68.735 | 1.00 28.46 |
| | ATOM | 4205 | CG | TYR B 153 | | 39.379 | -8.886 | 68.240 | 1.00 25.69 |
| | ATOM | 4206 | CD1 | TYR B 153 | | 38.618 | -8.560 -8.195 | 66.898 | 1.00 30.73 |
| | MOTA | 4207 | CEl | TYR B 153 | | 38.447 | -8.193 -8.847 | 67.856 | 1.00 24.82 |
| | ATOM | 4208 | CD3 | TYR B 153 | | 40.962 | -8.488 | 66.526 | 1.00 29.26 |
| | ATOM | ≟2 09 | CE2 | TYR B 153 | ٠ | 40.801 39.547 | -8.161 | 66.054 | 1.00 31.25 |
| | ATOM | 4210 | CZ | TYR B 153 | | 39.406 | -7.803 | 64.735 | 1.00 34.22 |
| | MOTA | 4211 | OH | TYR B 153 | | | -11.627 | 69.674 | 1.00 28.11 |
| | MOTA | 4212 | C | TYR- B 153 | | 39 975 | -12.248 | 68.759 | 1.00 22.06 |
| | ATOM | 4213 | 0 | TYR B 153 | | 41 310 | -11.725 | 69.944 | 1.00 26.77 |
| | ATOM | 4214 | N | LEU B 154 LEU B 154 | | 42.681 | -12.597 | 69.168 | 1.00 28.79 |
| | MOTA | 4215 | CA | LEU B 154 | | 44.142 | -12.386 | 69.592 | 1.00 28.06 |
| | ATOM | 4216 | CB CG | LEU B 154 | | 44.789 | -11.087 | 69.083 | 1.00 27.71 |
| | ATOM | 4217 | CD1 | | | 46.119 | -10.860 | 69.759 | 1.00 34.15 |
| | ATOM | 4218 4219 | CD2 | | | 44.968 | -11.171 | 67.571 | 1.00 26.71 |
| | ATOM | 4220 | C | LEU B 154 | | 42.299 | -14.074 | 69.274 | 1.00 25.98 |
| | MOTA MOTA | 4221 | Ö | LEU B 154 | | 42.282 | -14.787 | 68.271 | 1.00 29.88 1.00 23.19 |
| | ATOM | 1222 | N | ARG B 155 | | 41.996 | -14.536 | 70.480 | 1.00 29.47 |
| | ATOM | 4223 | CA | ARG B 155 | | 41.622 | -15.936 | 70.669 | 1.00 28.53 |
| | MOTA | 4224 | СB | ARG B 155 | | 41.339 | -16.230 | 72.144 | 1.00 35.03 |
| | ATOM | 4225 | CG | ARG B 155 | | 42.527 | -15.965 | 73.053 74.507 | 1.00 39.42 |
| | ATOM | 4226 | CD | ARG B 155 | | | -16.276 | 74.792 | _, , , |
| | ATOM | 4227 | NE | ARG B 155 | | 42.165 | -17.706 | 75.986 | |
| | ATOM | 4228 | CZ | ARG B 155 | | 41.869 | -18.209 -17.394 | 77.002 | 47 |
| | ATOM | 4229 | NH] | - | | 41.591 | -19.523 | 76.178 | |
| | MOTA | 4230 | | 2 ARG B 155 | | 40 303 41.012 | -16.260 | 69.832 | 1.00 29.07 |
| | ATOM | 4231 | | ARG B 155 | | 40.333 | -17.311 | 69.203 | 1.00 25.31 |
| | atom | 4232 | | ARG B 155 | | 30.J2J | -15.357 | 69.828 | 1.00 28.99 |
| • | ATOM | 4233 | | LYS B 156 | | 38 216 | -15.573 | | 1.00 34.63 |
| | ATOM | 4234 | | LYS B 156 LYS B 156 | | 37.148 | -14.534 | 69.386 | 1.00 36.63 |
| | ATOM | 1235 | | LYS B 156 | | 36.393 | -14.883 | 70.646 | |
| | ATOM | 4236 | | LYS B 156 | | 37.292 | -14.900 | 71.868 | |
| | ATCM | 4237 | | LYS B 156 | | 36.685 | -15.712 | 73.009 | |
| | MOTA | 1238 | | LYS B 156 | | 36.561 | 17.172 | 72.677 | |
| | ATOM | 4239 | | LYS B 156 | | 38.504 | -15.562 | 67.538 | |
| | ATOM | 4240 4241 | | LYS B 156 | | 37.722 | -16.088 | 66.754 | |
| | ATCM | 4242 | | LYS B 157 | | 39.625 | -14.966 | 67.140 | |
| | ATOM | 243 | | | | 39.996 | 5 -14.945 | 65.734 | |
| | ATOM | 1244 | | | | 40.888 | 3 -13.746 | 65.418 | |
| | atom atom | 4245 | | | | 40.157 | 7 -12.426 | 65.359 | 10 |
| | ATOM | 4246 | - | | | 39.132 | 2 -12.424 | 64.239 | 21 00 |
| | | | | | | 38.395 | 5 -11.103 | 64.17 | 1.00 52.50 |
| | ATOM | 747 | | | | | | | |

| | | 157 | 2 | 7 406 | -11.380 | 63.054 | 1.00 32.91 |
|------|------|----------------|--------|------------------|------------------------|----------|------------|
| ATOM | 4248 | NZ LYS B 157 | | | -16.234 | 65.381 | 1.00 31.92 |
| ATOM | 4249 | C LYS B 157 | | | | | 1.00 33.58 |
| ATOM | 4250 | O LYS B 157 | | | -16.421 | 64.246 | 1.00 28.97 |
| | 4251 | N GLY B 158 | | | -17.111 | 66.368 | 1.00 20.97 |
| ATOM | | 100 | 4 | 1.546 | -18.379 | 66.112 | 1.00 28.98 |
| ATOM | 4252 | | | | -18.569 | 66.622 | 1.00 33.33 |
| ATOM | 4253 | | | | -19.672 | 66.522 | 1.00 30.58 |
| ATOM | 4254 | O GLY B 158 | 4 | 3.303 | -17.521 | 67.164 | 1.00 32.80 |
| ATOM | 4255 | N PHE B 159 | 4 | 3.5/8 | -11.341 | 67.678 | 1.00 28.89 |
| ATOM | 4256 | CA PHE B. 159 | | | -17.657 | 67.076 | 1.00 30.33 |
| | 4257 | CB - PHE B 159 | 4 | 5.560 | -16.286 | 67,934 | 1.00 30.53 |
| MOTA | | CG PHE B 159 | 4 | 5.748 | -15.470 | 66.692 | 1.00 28:53 |
| MOTA | 4258 | CD1 PHE B 159 | 4 | 4.682 | -14.787 | 66.121 | 1.00 24.58 |
| MOTA | 4259 | | . 4 | 6 989 | -15.420 | 66.068 | 1.00 24.21 |
| ATOM | 4260 | | 4 | 1 219 | -14.066 | 64.948 | 1.00 25.26 |
| ATOM | 4261 | CE1 PHE B 159 | 7 | 7 160 | -14.706 | 64.895 | 1.00 23.66 |
| MOTA | 4262 | CE2 PHE B 159 | 4 | 7.100 | -14.026 | 64.332 | 1.00 26.65 |
| ATOM | 4263 | CZ PHE B 159 | 4 | 6.095 | -14.020 | 68.958 | 1.00 30.92 |
| ATOM | 4264 | C PHE B 159 | 4 | 4.969 | -18.484 | | 1.00 24.26 |
| ATOM | 4265 | O PHE B 159 | | | -18.334 | 69.820 | 1.00 28.86 |
| | 4266 | N LYS B 160 | 4 | 15.979 | -19.347 | 69.077 | 1.00 20.00 |
| ATOM | | CA LYS B 160 | 4 | 6.123 | | 70.237 | 1.00 30.27 |
| ATOM | 4267 | | 4 | 6.085 | -21.692 | 69.800 | 1.00 32.05 |
| ATOM | 4268 | | | 4.806 | _ | 69.113 | 1.00 41.13 |
| ATOM | 4269 | | | 4.809 | | 68.826 | 1.00 40.73 |
| ATOM | 4270 | CD LYS B 160 | | | | 67.904 | 1.00 43.16 |
| ATOM | 4271 | CE LYS B 160 | | 15.945 | | 66.554 | 1.00 48.69 |
| -TOM | 4272 | NZ LYS B 160 | • | 15.812 | -23.408 | | 1.00 28.23 |
| ATOM | 4273 | C LYS B 160 | | 47.394 | -19.997 | 71.048 | 1.00 25.29 |
| | 4274 | O LYS B 160 | | 47.552 | -20.561 | 72.130 | 1.00 23.23 |
| ATOM | 4275 | N ARG B 161 | | 48.320 | -19.206 | 70.520 | 1.00 28.51 |
| MOTA | 4213 | 1/1 | | 49.550 | -18.921 | 71.247 | 1.00 25.84 |
| ATOM | 4276 | 4.64 | | 50.724 | -19.719 | 70.667 | 1.00 25.33 |
| MOTA | 4277 | | • | 50 551 | -21.245 | 70.781 | 1.00 27.47 |
| ATOM | 4278 | | | 50.55 | -21.985 | 70.394 | 1.00 32.27 |
| MOTA | 4279 | CD ARG B 161 | | 51.033 51.033 | -21.761 | 69.002 | 1.00 34.90 |
| ATOM | 4280 | NE ARG B 161 | | 52.210 | 22.701 | 67.954 | 1.00 38.45 |
| ATOM | 4281 | CZ ARG B 161 | | 51.584 | -22.276 | | 1.00 38.77 |
| ATOM | 4282 | NH1 ARG B 161 | | 50.527 | -23.056 | 68.130 | 1.00 38.64 |
| | 4283 | NH2 ARG B 161 | | 51.999 | -22.000 | 66.725 | 1.00 30.40 |
| MOTA | 4284 | C ARG B 161 | | 49.818 | 3 -17.421 | 71.182 | 1.00 30.40 |
| ATOM | | O ARG B 161 | | 50.393 | -16.912 | 70.218 | 1.00 27.50 |
| ATOM | 4285 | 163 | | 49.376 | -16.722 | 72.221 | 1.00 25.64 |
| MOTA | 4286 | | | 49 515 | -15.273 | 72.303 | 1.00 27.44 |
| MOTA | 4287 | | | 4D.324 | 1 -14.618 | 72.545 | 1.00 24.53 |
| MOTA | 4288 | CB ILE B 162 | | 40.13 | -13.101 | 72.473 | 1.00 25.49 |
| ATOM | 4289 | CG2 ILE B 162 | | 40.24 | 2 -15.101 | 71.487 | 1.00 29.46 |
| ATOM | 4290 | CG1 ILE B 162 | | 47.14 | 2 -13.101 | 71.758 | 1.00 31.94 |
| ATOM | 4291 | CD1 ILE B 162 | | 45.68 | 8 -14.707 | 73.429 | 1.00 22.68 |
| ATOM | 4292 | C ILE B 162 | | 50.46 | 5 -14.868 | 73.449 | 1.00 24.25 |
| | 4293 | | | 5^.31 | 1 -15.302 | 74.568 | 1.00 24.25 |
| ATOM | 4294 | | | 545 | 4 -14.042 | 73.100 | 1.00 19.49 |
| ATOM | 4295 | | | 51.42 | 5 -13.561 | 74.081 | |
| atom | | | | 53.85 | 0 -13.686 | 73.528 | |
| ATOM | 4296 | | | 54 97 | 9 -12.975 | 74.295 | 1.00 18.84 |
| ATOM | 4297 | | | 55 10 | 2 -13.538 | | 1.00 20.55 |
| ATOM | 4298 | CD1 LEU B 16 | | 55.TO | 2 -13.330 3 -13.148 | | |
| ATOM | 4299 | CD2 LEU B 16 | , | 50.29 | 3 -13.190 | | |
| ATCM | 4300 | C LEU B 16 | } | 52.15 | 8 -12.099 | | |
| | 4301 | | } | 51.89 | 8 -11.277 | 73.549 | |
| ATOM | 4302 | | | 52.22 | 7 -11.780 | 75.715 | |
| ATOM | | | 1 | 52.02 | 7 -10.411 | 76.191 | |
| MOTA | 1303 | | - 1 | 50.77 | 7 -10.323 | 77.070 | 1.00 16.01 |
| ATOM | 4304 | | - 1 | 50.53 | | | 1.00 15.08 |
| ATOM | 4305 | CG TYR B 16 | 7 | 50.14 | | | 1.00 19.51 |
| ATOM | 4306 | | ± • | | | | 1.00 12.88 |
| ATOM | 4307 | | | 49.94 | | | |
| ATOM | 4308 | CD2 TYR B 16 | | 50.71 | 5 -8.724 | | |
| ATOM | 4309 |) CE2 TYR B 16 | | 50.52 | 0 -7.463 | | |
| | | | | 50.13 | 9 -6.40 | | |
| ATOM | 431 | | | 49.95 | 32 - 5.163 | 79.354 | 10 11 |
| ATOM | | | | 53.24 | 16 -10.01 | 77.018 | |
| ATOM | | | 4 | 53.53 | 9 -10.64 | 2 78.036 | 1.00 26.51 |
| ATOM | 431 | 3 O TAK B 10 | - | | | • | |
| • | | | | | | | |

| | | | | | E2 064 | -8.992 | 76.573 | 1.00 22.40 |
|--------------|--------------|---------|----------------|----------------|------------------|------------------|------------------|--------------------------|
| MOTA | 4314 | N 1 | LE B | 165 | 53.964 | -8.518 | 77.285 | 1.00 17.72 |
| ATOM | | | | 165 | 55.148 | -8.465 | 76.343 | 1.00 22.51 |
| ATOM | | | LE B | 165 | 56.352 | -7.902 | 77.079 | 1.00 16.36 |
| MOTA | | | | 165 | 57.582 | -9.880 | 75.818 | 1.00 19.82 |
| MOTA | | | LE B | 165 | 56.632 | -9.942 | 74.742 | 1.00 21.74 |
| ATOM | 4319 | | ILE B | 165 | 57.721 | -7.126 | 77.850 | 1.00 22.54 |
| ATOM | | | ILE B | 165 | 54.851 | -6.223 | 77.111 | 1.00 16.60 |
| ATOM | 4321 | 0 : | ILE B | 165 | 54.478 | -6.223 -6.961 | 79.156 | 1.00 15.78 |
| ATOM | 4322 | N I | ASP B | 166 | 55.046 | -5.704 | 79.840 | 1.00 20.62 |
| ATOM | 4323 | | ASP B | 166 | 54.740 | -5.996 | 80.949 | 1.00 17.57 |
| ATOM | 4324 | | ASP B | 166 | 53.719 | -4.742 | 81.486 | 1.00 25.39 |
| MOTA | | | ASP B | 166 | 53.063 53.779 | -3.859 | 82.003 | 1.00 19.68 |
| MOTA | 4326 | OD1 . | ASP B | 166 | 51.824 | -4.637 | 81.377 | 1.00 29.22 |
| MOTA | 4327 | | ASP B | | 55.976 | -5.002 | 80.423 | 1.00 19.01 |
| MOTA | 4328 | | ASP B | | 56.509 | -5.412 | 81.456 | 1.00 19.74 |
| ATOM | 4329 | | ASP B | | 56.414 | -3.923 | 79.775 | 1.00 17.88 |
| MOTA | 4330 | | LEU B | | 57.598 | -3.211 | 80.235 | 1.00 14.99 |
| MOTA | 4331 | | LEU B LEU B | 167 | 58.412 | -2.710 | 79.044 | 1.00 19.22 |
| MOTA | 4332 | | | | 58.871 | -3.799 | 78.069 | 1.00 22.68 |
| MOTA | 4333 | | LEU B | | 59.835 | -3.179 | 77.074 | 1.00 25.35 |
| MOTA | 4334 | | | | 59.570 | -4.943 | 78.808 | 1.00 17.54 |
| MOTA | 4335 | | LEU B | | 57.284 | -2.059 | 81.183 | 1.00 17.49 |
| MOTA | 4336 | | LEU B | | 58.189 | -1.359 | 81.639 | 1.00 13.39 |
| MOTA | 4337 | | ASP S | | 56.003 | -1.878 | 81.479 | 1.00 20.03 |
| MOTA | 4338 | N | ASP E | | 55.549 | -0.848 | 82.412 | 1.00 21.98 |
| MOTA | 4339 | CA | ASP E | | 54.030 | -0.955 | 82.597 | 1.00 21.21 |
| MOTA | 4340 | CB | ASP E | | 53.453 | 0.186 | 83.428 | 1.00 24.92 |
| ATOM | 4341 | CG C | ASP E | | 56.241 | -1.139 | 83.753 | 1.00 22.98 |
| ATOM | 4342 | 0 | ASP E | | 56.447 | -2.304 | 84.091 | 1.00 18.36 |
| ATOM | 4343 | | ASP E | | 52.849 | 1.099 | 82.825 | 1.00 22.03 |
| MOTA | 4344 4345 | OD2 | ASP E | | 53.606 | 0.189 | 84.676 | 1.00 18.43 |
| MOTA | 4345 | N | ALA E | | 56.581 | -0.095 | 84.514 | 1.00 15.46 |
| MOTA | 4347 | CA | ALA I | | 57.263 | -0.∙268 | 85.807 | 1.00 18.73 |
| ATOM | 4348 | CB | ALA I | | 57.764 | 1.084 | 86.323 | 1.00 11.98 |
| ATOM ATOM | 4349 | c | ALA I | | 56.400 | -0.940 | 86.886 | 1.00 21.82 |
| MOTA | 4350 | ō | ALA I | | 56.886 | -1.262 | 87.980 | 1.00 22.51 1.00 18.75 |
| ATOM | 4351 | N | HIS I | | 55.120 | | 86.600 | 1.00 18.73 |
| ATOM | 4352 | CA | HIS 1 | в 170 | 54.238 | -1.776 | 87.570 87.015 | 1.00 22.75 |
| MOTA | 4353 | C | HIS 3 | в 170 | 53.716 | | 87.013 | 1.00 21.94 |
| ATOM | 4354 | 0 | HIS ! | | 53.536 | | 87.927 | 1.00 21.28 |
| ATOM | 4355 | CB | HIS : | | 53.050 | | 88.460 | 1.00 18.89 |
| MOTA | 4356 | CG | | В 170 | 53.449 | | 87.626 | 1.00 19.13 |
| ATOM | 4357 | ND1 | | в 170 | 53.695 | | 88.412 | 1.00 19.41 |
| ATOM | 4358 | CE1 | HIS | B 170 | 54.046 53.660 | | 89.746 | 1.00 19.02 |
| MOTA | 4359 | CD2 | HIS | B 170 | 54.042 | | 89.710 | 1.00 20.45 |
| ATOM | 4360 | NE2 | HIS | B 170 | 53.474 | | 87.907 | 1.00 19.20 |
| ATOM | 4361 | N | HIS | B 171 | 52.961 | | 87.519 | 1.00 21.20 |
| ATOM | 4362 | CA | HIS | B 171 | 52.964 | | | 1.00 22.00 |
| MOTA | 4363 | CB | HIS | B 171 | 52.541 | | | 1.00 24.64 |
| ATOM | 4364 | CG | HIS | B 171 | 53.056 | | | 1.00 19.19 |
| MOTA | 4365 | CD2 | HIS | B 171 | 51.441 | | | 1.00 25.71 |
| MOTA | 4366 | NDI | HIS | B 171 | 51.295 | | | 1.00 25.30 |
| MOTA | 4367 | CEI | HIS | B 171 | 52.261 | | | 1.00 24.71 |
| MOTA | 4368 | | HIS | B 171 | 51.549 | | | 1.00 23.91 |
| MOTA | 4369 | Ċ | HIS | B 171 | 50.67 | | | 1.00 18.93 |
| MOTA | 4370 | 0 | HTD | B 171 | 51.33 | | 85.865 | |
| atom | 4371 | N | CIS | В 172 В 172 | 50.03 | | 85.207 | 1.00 20.03 |
| ATOM | 4372 | CA | CYS | B 172 | 50.24 | | 83.732 | 1.00 22.46 |
| ATOM | 4373 | CB | | B 172 | 51.25 | | 83.419 | 1.00 23.49 |
| ATOM | 4374 | SG | CVE | B 172 | 49.11 | | 85.913 | |
| ATOM | 4375 | | CVS | B 172 | 48.71 | | L 85.327 | 1.00 18.23 |
| ATOM | 4376 | | 255 | B 173 | 48.76 | | L 87.170 | |
| ATOM | 1377 | | 7CD | B 173 | 47.90 | 9 -7.776 | 5 87.928 | 1.00 18.81 |
| ATOM | 1378 1379 | | 76b | B 173 | 47.63 | | 5 89.344 | 1.00 20.39 |
| ATCM | <u>:</u> 379 | | A)E | | | | - | |
| | | | | | | | | |

| ATOM | 4380 | CG ASP B 173 | | | 00 23.40 |
|--------------|--------------|-------------------------------|-----------------------------------|----------------------|--------------------------|
| ATOM | 4381 | OD1 ASP B 173 | 46.564 -5.435 | | 00 18.64 00 19.24 |
| ATOM | 4382 | OD2 ASP B 173 | 46.834 -5.231 | | 00 17.46 |
| ATOM | 4383 | C ASP B 173 | 46.595 -8.116 | | 00 15.53 |
| MOTA | 4384 | O ASP B 173 | 46.162 -9.272 | | 00 13.46 |
| ATOM | 4385 | N GLY B 174 | 45.978 -7.130 | | 00 18.18 |
| ATOM | 4386 | CA GLY B 174 | 44.733 -7.391 44.904 -8.392 | 84.741 1. | 00 17.85 |
| ATOM | 4387 | C GLY B 174 | 44.904 -8.392 44.104 -9.316 | | 00 18.27 |
| MOTA | 4388 | O GLY B 174 | 45.951 -8.214 | | 00 16.14 |
| ATOM | 4389 | N VAL B 175 CA VAL B 175 | 46.206 -9.111 | 82.829 1. | .00 17.00 |
| MOTA | 4390 | | 47.305 -8.552 | 81,902 1. | .00 27.22 |
| ATOM | 4391 | CB VAL B 175 CG1 VAL B 175 | 47.533 -9.507 | | .00 19.75 |
| ATOM | 4392 4393 | CG2 VAL B 175 | 46.896 -7.169 | | .00 18.66 |
| MOTA | 4394 | C VAL B 175 | 46.635 -10.486 | | .00 22.82 |
| ATOM ATOM | 4395 | O VAL B 175 | 46.255 -11.503 | | .00 18.06 |
| ATOM | 4396 | N GLN B 176 | 47.439 -10.520 | | .00 21.67 .00 21.55 |
| ATOM | 4397 | CA GLN B 176 | 47.889 -11.798 | - | .00 19.68 |
| MOTA | 4398 | CB GLN B 176 | 48.824 -11.602 | 86.105 1 86.862 1 | .00 20.17 |
| ATOM | 4399 | CG GLN B 176 | 49.088 -12.905 | 87.996 1 | .00 25.42 |
| MOTA | 4400 | CD GLN B 176 | 50.066 -12.759 51.243 -12.442 | | .00 21.56 |
| MOTA | 4401 | OE1 GLN B 176 | 49.592 -13.000 | | .00 20.18 |
| MOTA | 4402 | NE2 GLN B 176 C GLN B 176 | 46.689 -12.630 | 85.348 1 | .00 24.78 |
| MOTA | 4403 | 7 176 | 46.618 -13.817 | 85.057 1 | .00 22.91 |
| MOTA | 4404 | O GLN B 176 N GLU B 177 | 45.751 -12.007 | | .00 23.69 |
| ATOM | 4405 4406 | CA GLU B 177 | 44.571 -12.727 | | .00 27.01 |
| MOTA | 4407 | CB GLU B 177 | 43.703 -11.825 | • | .00 24.73 |
| MOTA MOTA | 4408 | CG GLU B 177 | 42.633 -12.581 | | .00 37.46 |
| MOTA | 4409 | CD GLU B 177 | 41.767 -11.676 | | .00 42.48 .00 44.35 |
| ATOM | 4410 | OE1 GLU B 177 | 40.875 -11.002 | | .00 45.63 |
| ATOM | 4411 | OE2 GLU B 177 | 41.993 -11.627 | | .00 26.56 |
| ATOM | 4412 | C GLU B 177 | 43.732 -13.247. 43.240 -14.375 | 85.408 1 | 00 27.71 |
| ATOM | 4413 | O GLU B 177 | 43.573 -12.418 | | .00 24.58 |
| ATOM | 4414 | N ALA B 178 | 42.776 -12.775 | | 00 25.86 |
| MOTA | 4415 | CA ALA B 178 CB ALA B 178 | 42.778 -11.628 | | 00 24.20 |
| MOTA | 4416 | CB ALA B 178 C ALA B 178 | 43.231 -14.054 | | 00 25.72 |
| MOTA MOTA | 4417 4418 | O ALA B 178 | 42.406 -14.838 | | 00 22.38 |
| MOTA | 4419 | N PHE B 179 | 44.535 -14.282 | | 1.00 27.19 1.00 27.05 |
| ATOM | 4420 | CA PHE B 179 | 44.990 -15.489 | | 1.00 27.03 |
| ATOM | 4421 | CB PHE B 179 | 45.714 -15.086 | | 1.00 20.36 |
| ATOM | 4422 | CG PHE B 179 | 44.992 -14.020 | | 1.00 25.23 |
| ATOM | 4423 | CD1 PHE B 179 | 45.387 -12.687 43.860 -14.332 | 78.902 | 1.00 19.22 |
| ATOM | 4424 | CD2 PHE B 179 | 44.659 -11.677 | 79.102 | 1.00 19.25 |
| ATOM | 4425 | CE1 PHE B 179 | 43.128 -13.315 | 78.272 | 1.00 20.65 |
| MOTA | 4426 | CE2 PHE B 179 CZ PHE B 179 | 43.528 -12.001 | 78.374 | 1.00 25.64 |
| MOTA | 4427 | CZ PHE B 179 C PHE B 179 | 45.866 -16.398 | 82.556 | 1.00 23.50 |
| ATOM | 4428 4429 | O PHE B 179 | 46.652 -17.182 | | 1.00 18.26 |
| ATOM | 1430 | N TYR B 180 | 45.689 -16.313 | | 1.00 23.24 |
| MOTA MOTA | 4431 | CA TYR B 180 | 46.479 -17.106 | • • • • • • | 1.00 26.76 1.00 25.72 |
| ATOM | 4432 | CB TYR B 180 | 46.150 -16.665 | | 1.00 29.66 |
| MOTA | 4433 | CG TYR B 180 | 47.226 -16.969 | • | 1.00 27.07 |
| MOTA | 4434 | CD1 TYR B 180 | 47.037 -17.942 | 88.237 89.170 | 1.00 30.08 |
| ATOM | 4435 | CE1 TYR B 180 | 48.039 -18.222 48.444 -16.283 | 87.216 | 1.00 29.68 |
| MOTA | 4436 | CD2 TYR B 180 | 49.451 -16.552 | 88.139 | 1.00 30.99 |
| ATCM | 4437 | CE2 TYR B 180 | 49.431 -16.532 | 89.112 | 1.00 33.16 |
| ATOM | 4438 | | 50.262 -17.791 | 90.006 | 1.00 28.47 |
| ATOM | 1439 | 100 | 46.256 -18.619 | 84.649 | 1.00 29.13 |
| ATOM | 4440 | 100 | 47.163 -19.416 | | 1.00 23.43 |
| ATOM | 4441 4442 | | 45.073 -19.021 | 84.190 | 1.00 25.67 |
| ATOM | 4443 | | 44.784 -20.445 | 84.075 | 1.00 28.28 |
| ATOM ATOM | 1444 | CB ASP B 181 | 43.446 -20.759 | 84.757 | 1.00 32.13 1.00 36.12 |
| ATCM | 1445 | 101 | 42.247 -20.410 | 83.890 | 1.00 00.12 |

```
42.202 -19.300 83.329
41.334 -21.249 83.782
                                                               1.00 41.04
       4446 OD1 ASP B 181
MOTA
                                                               1.00 44.36
              OD2 ASP B 181
       4447
MOTA
                                                      82.664
                                    44.773 -21.018
                                                               1.00 32.41
                   ASP B 181
ATOM
        4448
              C
                                    44.246 -22.115
                                                      82.444
                                                               1.00 31.67
                   ASP B 181
        4449
              0
MOTA
                                                      81.702
                                                               1.00 29.24
                                   45.345 -20.302
                   THR B 182
        4450
              N
MOTA
                                                              1.00 30.57
1.00 30.03
                                   45.363 -20.823
44.468 -20.008
                                                      80.340
                   THR B 182
        4451
              CA
MOTA
                                                      79.397
              CB THR B 182
OG1 THR B 182
        4452
ATOM
                                    44.516 -20.598
44.947 -18.561
46.759 -20.870
                                                              1.00 28.22
                                                      78.095
ATOM
        4453
                                                               1.00 26.55
                                                      79.310
              CG2 THR B 182
        4454
ATOM
                                                               1.00 32.31
                                                      79.740
                   THR B 182
        4455
ATOM
                                                               1.00 27.27
                                    47.591 -20.007
                                                      80.008
                   THR B 182
        4456
              0
MOTA
                                                               1.00 29.94
                                    46.999 -21.878
                                                      78.909
                   ASP B 183
        4457
              N
MOTA
                                                      78.273
                                                               1.00 31.40
                                    48.296 -22.049
                  ASP B 183
        4458
              CA
MOTA
                                                               1.00 33.36
                                    48.648 -23.536
                                                      78.228
                  ASP B 183
              CB
        4459
MOTA
                                    47.718 -24.319
46.513 -23.988
                                                      77.328
                                                               1.00 33.33
              CG ASP B 183
        4460
MOTA
                                                      77.287
                                                               1.00 28.06
               OD1 ASP B 183
        4461
ATOM
                                    48.186 -25.271
                                                               1.00 38.19
                                                      76.675
              OD2 ASP B 183
        4462
MOTA
                                                               1.00 31.14
1.00 28.74
                                                      76.864
                                    48.321 -21.462
        4463
                   ASP B 183
               С
ATOM
                                    49.332 -21.557
                                                      76.168
                   ASP B 183
        4464
               0
                                                               1.00 25.34
ATOM
                                    47.217 -20.852 76.446 1.00 25.34
47.151 -20.251 75.118 1.00 28.59
45.712 -20.256 74.581 1.00 26.84
                   GLN B 184
        4465
               N
MOTA
                   GLN B 184
        4466
               CA
MOTA
                   GLN B 184
        4467
               CB
ATOM
                                    45.060 -21.632
                                                               1.00 34.86
                                                      74.529
                   GLN B 184
               CG
        4468
ATOM
                                                               1.00 32.27
                                    43.760 -21.647
                                                      73.736
                   GLN B 184
        4469
               CD
ATOM
                                    42.897 -20.789 73.912
43.611 -22.641 72.870
                                                                1.00 35.43
               OE1 GLN B 184
        4470
MOTA
                                    43.611 -22.641
47.672 -18.817
47.871 -18.171
                                                                1.00 28.92
              NE2 GLN B 184
        4471
MOTA
                                                      75.175
                                                                1.00 27.28
                    GLN B 184
        4472
              С
ATOM
                                                                1.00 29.70
                                                      74.148
                    GLN B 184
        4473
              0
ATOM
                                                      76.386
                                                                1.00 27.64
                                    47.900 -18.325
              N
                    VAL B 185
        4474
 ATOM
                                                      76.575
                                                                1.00 26.26
                                     48.400 -16.972
                    VAL B 185
         4475
              CA
 MOTA
                                     47.304 -16.039 77.145
47.879 -14.642 77.395
46.136 -15.967 76.191
                                                                1.00 22.85
                   VAL B 185
         4476
              CB
 MOTA
                                                                1.00 23.10
               CG1 VAL B 185
         4477
 MOTA
                                                                1.00 21.67
               CG2 VAL B 185
         4478
 MOTA
                                                                1.00 27.01
                                     49.570 -16.964 77.547
                    VAL B 185
VAL B 185
               C
         4479
 ATOM
                                     49.456 -17.469 78.663
                                                                1.00 23.75
         4480
               0
                                     50.696 -16.403 77.115
51.868 -16.301 77.978
53.142 -16.763 77.252
 ATOM
                                                                1.00 22.02
                    PHE B 186
         4481
               N
 ATOM
                                                                1.00 21.83
                   PHE B 186
               CA
         4482
 MOTA
                                                                1.00 17.02
                   PHE B 186
         4483
               CB
 MOTA
                                                                1.00 24.84
                                     54.336 -16.921
                                                      78.170
                    PHE B 186
         4484
               CG
                                                                1.00 22.70
1.00 20.26
 ATOM
                                                       78.580
                                     54.756 -18.189
               CD1 PHE B 186
         4485
 MOTA
                                     55.004 -15.805
                                                       78.670
               CD2 PHE B 186
         4486
                                                                1.00 21.47
 ATOM
                                                       79.471
                                     55.819 -18.338
               CE1 PHE B 186
         4487
 MOTA
                                                                1.00 20.01
                                                       79.563
                                     56.071 -15.941
56.481 -17.206
               CE2 PHE B 186
         4488
 ATOM
                                                                1.00 17.84
                                                       79.968
                    PHE B 186
         4489
               CZ
 MOTA
                                                                1.00 18.12
                                     52.032 -14.827
                                                       78.368
                    PHE B 186
         4490
              C
 ATOM
                                                                1.00 15.92
                                                       77.508
                                     52.038 -13.946
                                                                1.00 18.06
                    PHE B 186
               0
         4491
 ATO:
                                                       79.661
                                     52.161 -14.565
                    VAL B 187
               N
         4492
                                                                1.00 17.67
 ATO.4
                                     52.348 -13.208
                                                       80.153
               CA VAL B 187
         4493
 ATOm
                                                                1.00 22.85
                                     51.282 -12.839
51.608 -11.473
                                                       81.225
                    VAL B 187
         4494
               CB
 MOTA
                                                                1.00 24.08
                                                       81.840
         4495 CG1 VAL B 187
 MOTA
                                                       80.598. 1.00 18.82
                                     49.882 -12.808
              CG2 VAL B 187
         1496
 MOTA
                                                                1.00 18.32
                                                       80.788
                                     53.735 -13.060
         4497
               С
                    VAL B 187
 MOTA
                                                        81.707
                                                                 1.00 18.82
                                     54.092 -13.807
                    VAL B 187
         4498
               0
                                                                1.00 14.70
 MOTA
                                                        80.282
                                     54.503 -12.103
                    LEU B 188
         4499
               N
 ATCM
                                     55.832 -11.789
56.900 -11.948
                                                                1.00 18.84
                                                        80.798
                    LEU B 188
         4500
               CA
 MOTA
                                                        79.716
                                                                1.00 18.64
                    LEU B 188
         4501
               CB
  ATCM
                                                        80.082 1.00 21.23
                                     58.230 -11.277
                    LEU B 188
                                                                1.00 18.55
         4502
                CG
  MOTA
                                                        81.395
                                     58.769 -11.832
               CD1 LEU B 188
         4503
  ATOM
                                                                 1.00 20.49
                                                        78.957
                                      59.227 -11.489
               CD2 LEU B 188
         4504
  MOTA
                                                                1.00 22.14
                                     55.836 -10.339
                                                        81.280
                     LEU B 188
         4505
                                                                 1.00 19.96
  ATCM
                                                        80.517
                                              -9.410
                                      55.527
                    LEU B 188
          ≟506
                0
  ATOM
                                                                1.00 21.08
                                                        82.540
                                      56.187 -10.133
                     SER B 189
                N
         ₹507
                                                                1.00 21.85
  ATOM
                                                        83.061
                                              -8.782
                                      56.203
                     SER B 189
          4508 CA
                                                        83.908 1.00 25.95
 - ATOM
                                      54.956
                                              -8.543
                     SER B 189
          4509
               CB
                                                                 1.00 21.91
  ATOM
                                                        84.475
                                      54.988
                                              -7.252
                     SER B 189
          4510 OG
  ATCM
                                                        83.883 1.00 23.62
                                      57.423 -8.420
                     SER B 189
          4511 C
  ATOM
```

| | | | • | | | |
|------|-------|---------------|--------|--------|--------|-------------------|
| | | o SER B 189 | 57.829 | -9.174 | 84.766 | 1.00 18.61 |
| ATOM | 4512 | | 58.020 | | 83.569 | 1.00 20.33 |
| ATOM | 4513 | N LEU B 190 | | | | 1.00 21.85 |
| MOTA | 4514 | CA LEU B 190 | 59.149 | | | 1.00 22.85 |
| ATOM | 4515 | CB LEU B 190 | 60.278 | | 83.473 | |
| | 4516 | CG LEU B 190 | 60.964 | | 82.413 | 1.00 32.59 |
| ATOM | | CD1 LEU B 190 | 62.337 | -6.479 | 82.140 | 1.00 29.27 |
| MOTA | 4517 | CDI LEG B 190 | 61.136 | -8.511 | 82.379 | 1.00 31.98 |
| MOTA | 4518 | CD2 LEU B 190 | 58.505 | | 85.085 | 1.00 21.28 |
| MOTA | 4519 | C LEU B 190 | | | 84.501 | 1.00 15.72 |
| ATOM | 4520 | O LEU B 190 | 57.695 | | | 1.00 18.16 |
| ATOM | 4521 | N _ HIS B 191 | 58.857 | -5.421 | 86.351 | |
| | 4522 | CA HIS B 191 | 58.249 | -4.357 | 87.145 | 1.00 17.46 |
| ATOM | | CB HIS B 191 | 56.759 | -4.690 | 87.369 | 1.00 16.00 |
| MOTA | 4523 | | 56.517 | -6.085 | 87.880 | 1.00 22.14 |
| MOTA | 4524 | | 56.341 | -6.551 | 89.143 | 1.00 12.25 |
| MOTA | 4525 | | 56.372 | -7.179 | 87.049 | 1.00 18.02 |
| MOTA | 4526 | ND1 HIS B 191 | | -8.256 | 87.775 | 1.00 8.17 |
| MOTA | 4527 | CE1 HIS B 191 | 56.119 | | 89.049 | 1.00 19.79 |
| ATOM | 4528 | NE2 HIS B 191 | 56.094 | -7.902 | | |
| ATOM | 4529 | C HIS B 191 | 58.945 | -4.197 | 88.484 | |
| | 4530 | O HIS B 191 | 59.769 | -5.029 | 88.867 | 1.00 18.74 |
| ATOM | 4531 | N GLN B 192 | 58.618 | -3.114 | 89.182 | 1.00 18.20 |
| MOTA | | | 59.173 | -2.854 | 90.502 | 1.00 18.41 |
| MOTA | 4532 | | 58.690 | -1.500 | 91.034 | 1.00 20.71 |
| ATOM | 4533 | | 58.871 | -0.334 | 90.072 | 1.00 21.49 |
| MOTA | 4534 | CG GLN B 192 | | 0.930 | 90.594 | 1.00 20.65 |
| ATOM | 4535 | CD GLN B 192 | 58.226 | | 91.459 | 1.00 21.52 |
| ATOM | 4536 | OE1 GLN B 192 | 58.775 | 1.615 | | 1.00 15.10 |
| ATOM | 4537 | NE2 GLN B 192 | 57.029 | 1.226 | 90.098 | |
| ATOM | 4538 | C GLN B 192 | 58.608 | -3.945 | 91.395 | 1.00 17.55 |
| | 4539 | O GLN B 192 | 57.415 | -4.256 | 91.320 | 1.00 17.48 |
| ATOM | | 100 | 59.447 | -4.522 | 92.240 | 1.00 15.71 |
| ATOM | 4540 | 103 | 58.986 | -5.574 | 93.143 | 1.00 20.58 |
| ATOM | 4541 | 403 | 60.093 | -5.963 | 94.120 | 1.00 20.71 |
| MOTA | 4542 | CB SER B 193 | | -6.804 | 95.138 | 1.00 22.55 |
| ATOM | 4543 | OG SER B 193 | 59.571 | | 93.947 | 1.00 21.31 |
| ATOM | 4544 | C SER B 193 | 57.774 | -5.112 | | 1.00 20.82 |
| ATOM | 4545 | O SER B 193 | 57.769 | -4.003 | 94.486 | 1.00 21.80 |
| ATOM | 4546 | N PRO B 194 | 56.745 | -5.967 | 94.063 | |
| | 4547 | CD PRO B 194 | 56.648 | -7.331 | 93.524 | 1.00 24.27 |
| ATOM | 4548 | CA PRO B 194 | 55.524 | -5.643 | 94.812 | 1.00 23.58 |
| ATOM | | | 54.678 | -6.909 | 94.642 | 1.00 22.98 |
| MOTA | 4549 | | 55.168 | -7.458 | 93.317 | 1.00 26.35 |
| ATOM | 4550 | | 55.841 | -5.366 | 96.283 | 1.00 25.79 |
| MOTA | 4551 | C PRO B 194 | 55.009 | -4.831 | 97.022 | 1.00 27.26 |
| ATOM | 4552 | O PRO B 194 | | -5.736 | 96.710 | 1.00 23.20 |
| ATOM | 4553 | N GLU B 195 | 57.045 | | 98.093 | 1.00 29.56 |
| ATOM | 4554 | CA GLU B 195 | 57.428 | -5.514 | | 1.00 32.38 |
| ATOM | 4555 | CB GLU B 195 | 58.816 | -6.090 | 98.379 | 1.00 32.35 |
| | 4556 | CG GLU B 195 | 58.940 | -7.567 | 98.049 | |
| ATOM | | CD GLU B 195 | 60.206 | -8.189 | 98.613 | 1.00 50.44 |
| ATOM | 4557 | OE1 GLU B 195 | 61.290 | -7.580 | 98.471 | <u>:.00 50.51</u> |
| MOTA | 4558 | OE2 GLU B 195 | 60.118 | -9.297 | 99.184 | 1.00 49.77 |
| MOTA | 4559 | 105 | 57.414 | -4.035 | 98.425 | 1.00 25.11 |
| ATOM | 4560 | C GLU B 195 | 57.095 | -3.659 | 99.551 | 1.00 29.05 |
| ATOM | 4561 | O GLU B 195 | | -3.191 | 97.445 | 1.00 22.90 |
| ATOM | 4562 | N TYR B 196 | 57.729 | | 97.696 | 1.00 22.46 |
| ATOM | 4563 | CA TYR B 196 | 57.743 | -1.750 | | 1.00 22.72 |
| ATCM | 4564 | 100 | 59.188 | -1.223 | 97.668 | 1.00 22.72 |
| | .4565 | 100 | 59.855 | -1.234 | 96.301 | 1.00 24.17 |
| ATOM | | | 59.639 | -0.203 | 95.385 | 1.00 20.87 |
| MOTA | 4566 | | 60.229 | -0.222 | 94.118 | 1.00 18.31 |
| MOTA | 4567 | 100 | 60.684 | -2.289 | 95.916 | 1.00 24.63 |
| ATOM | 4568 | | 61.276 | -2.318 | 94.648 | 1.00 24.39 |
| ATOM | 4569 | | 01.4/0 | | 93.756 | 1.00 23.01 |
| ATOM | 4570 | CZ TYR B 196 | 61.042 | -1.284 | | 1.00 19.86 |
| ATOM | 4571 | 100 | 61.592 | -1.328 | 92.492 | 1.00 23.54 |
| | 4572 | | 56.896 | | 96.725 | 1.00 17.53 |
| ATOM | | | 56.779 | 0.275 | 96.869 | 1.00 11.33 |
| ATOM | 4573 | | 56.293 | -1.589 | 95.740 | 1.00 22.11 |
| ATOM | 4574 | | 55.503 | | 94.779 | 1.00 24.28 |
| ATOM | 4575 | | 56.310 | | | 1.00 23.03 |
| ATOM | 4576 | CB ALA B 197 | | | | |
| MOTE | 4577 | C ALA B 197 | 54.153 | -1.412 | | - |

| | | ^ | ALA B 197 | | 53.910 | -2.609 | 94.549 | 1.00 17.67 |
|------|------|------|------------------------|---|--------|------------------|------------------|------------|
| MOTA | 4578 | 0 | PHE B 198 | | 53.278 | -0.541 | 93.932 | 1.00 26.40 |
| ATOM | 4579 | N | PHE B 198 | | 51.956 | -0.950 | 93.495 | 1.00 28.19 |
| ATOM | 4580 | CA | | | 51.152 | 0.263 | 93.035 | 1.00 29.51 |
| MOTA | 4581 | СВ | PHE B 198 | | 49.721 | -0.050 | 92.711 | 1.00 29.50 |
| MOTA | 4582 | CG | PHE B 198 | | 48.732 | 0.100 | 93.674 | 1.00 32.77 |
| MOTA | 4583 | CD1 | PHE B 198 | | 49.367 | -0.533 | 91.455 | 1.00 25.82 |
| MOTA | 4584 | | PHE B 198 | | | -0.223 | 93.394 | 1.00 36.70 |
| ATOM | 4585 | CEl | PHE B 198 | | 47.410 | -0.223 | 91.170 | 1.00 29.29 |
| ATOM | 4586 | CE2 | PHE B.198 | | 48.050 | | 92.141 | 1.00 33.05 |
| ATOM | 4587 | CZ | PHE B 198 | | 47.071 | -0.703 | 92.284 | 1.00 28.28 |
| ATOM | 4588 | С | PHE B 198 | | 52.170 | -1.858 | 91.456 | 1.00 27.15 |
| MOTA | 4589 | 0 | PHE B 198 | | 53.045 | -1.602 | 92.185 | 1.00 31.37 |
| ATOM | 4590 | N | PRO B 199 | | 51.407 | -2.952 | 91.045 | 1.00 37.07 |
| ATOM | 4591 | CD | PRO B 199 | | 51.440 | -3.887 | 93.144 | 1.00 35.32 |
| ATOM | 4592 | CA | PRO B 199 | | 50.386 | -3.369 | 92.321 | 1.00 33.88 |
| ATOM | 4593 | CB | PRO B 199 | | 49.545 | -4.328 | 91.578 | 1.00 36.75 |
| MOTA | 4594 | CG | PRO B 199 | | 50.641 | -5.068 | 94.184 | 1.00 36.93 |
| ATOM | 4595 | С | PRO B 199 | | 51.241 | -4.082 | 93.860 | 1.00 50.93 |
| ATOM | 4596 | 0 | PRO B 199 | | 52.308 | -4.603 | 95.422 | 1.00 37.04 |
| ATOM | 4597 | N | PHE B 200 | | 50.804 | -4.127 | | 1.00 30.13 |
| ATOM | 4598 | CA | PHE B 200 | | 51.644 | -4.763 | 96.421 97.723 | 1.00 28.70 |
| ATOM | 4599 | CB | PHE B 200 | | 51.547 | -3.968 | | 1.00 29.98 |
| ATOM | 4600 | CG | PHE B 200 | | 51.760 | -2.485 | 97.543 | 1.00 28.92 |
| ATOM | 4601 | CD1 | PHE B 200 | | 50.717 | -1.660 | 97.137 | 1.00 28.92 |
| MOTA | 4602 | CD2 | PHE B 200 | | 53.016 | -1.919 | 97.746 | 1.00 23.60 |
| MOTA | 4603 | CE1 | PHE B 200 | | 50.922 | -0.289 | 96.938 | 1.00 27.05 |
| MOTA | 4604 | CE2 | PHE B 200 | | 53.229 | -0.558 | 97.547 | 1.00 23.30 |
| MOTA | 4605 | CZ | PHE B 200 | | 52.182 | 0.260 | 97.143 | 1.00 25.51 |
| ATOM | 4606 | С | PHE B 200 | | 51.296 | -6.227 | 96.658 | 1.00 20.92 |
| ATOM | 4607 | 0 | PHE B 200 | | 52.112 | -6.984 | 97.167 | 1.00 20.32 |
| ATOM | 4608 | N | GLU B 201 | | 50.094 | -6.618 | 96.252 | 1.00 31.98 |
| ATOM | 4609 | CA | GLU B 201 | | 49.576 | -7.972 | 96.454 96.487 | 1.00 31.57 |
| MOTA | 4610 | CB | GLU B 201 | | 48.056 | -7.928 | | 1.00 39.17 |
| ATOM | 4611 | CG | GLU B 201 | | 47.486 | -6:935 | 97.449 97.316 | 1.00 40.31 |
| ATOM | 4612 | CD | GLU B 201 | | 45.987 | -6.853 | 97.500 | 1.00 38.90 |
| ATOM | 4613 | OE: | | | 45.332 | -7.902 -5.751 | 97.019 | 1.00 35.04 |
| MOTA | 4614 | OE | | | 45.475 | -9.018 | 95.422 | 1.00 30.83 |
| MOTA | 4615 | С | GLU B 201 | | 49.979 | -10.219 | 95.690 | 1.00 26.34 |
| MOTA | 4616 | 0 | GLU B 201 | | 50.362 | -8.573 | 94.234 | 1.00 24.95 |
| MOTA | 4617 | N | LYS B 202 | | 50.764 | -9.501 | 93.195 | 1.00 22.79 |
| ATOM | 4618 | CA | LYS B 202 | | 49.588 | -9.773 | 92.258 | 1.00 25.12 |
| ATOM | 4619 | CB | LYS B 202 | | | -10.523 | 93.000 | 1.00 35.38 |
| MOTA | 4620 | CG | LYS B 202 | | 40.404 | -11.099 | 92.103 | 1.00 38.67 |
| MOTA | 4621 | CD | LYS B 202 | | 46 498 | -11.998 | 92.903 | 1.00 40.98 |
| MOTA | 4622 | CE | | | 45 491 | -12.659 | 92.028 | 1.00 46.65 |
| MOTA | 4623 | | LYS B 202 LYS B 202 | | 51.975 | -9.007 | 92.435 | 1.00 24.62 |
| MOTA | 4624 | C | LYS B 202 | | 52.355 | -7.838 | 92.549 | 1.00 21.83 |
| MOTA | 4625 | 0 | GLY B 203 | | 52.598 | | | 1.00 17.60 |
| MOTA | 4626 | | | | 53.779 | | | 1.00 19.41 |
| MOTA | 4627 | | GLY B 203 | | 55.014 | -10.297 | | 1.00 20.36 |
| MOTA | 4628 | | GLY B 203 | | 56.101 | -10.070 | 90.888 | 1.00 23.83 |
| MOTA | 4629 | | PHE B 204 | | 54.855 | -11.201 | 92.358 | 1.00 24.82 |
| MOTA | 4630 | | | | 55.992 | -11.957 | 92.859 | 1.00 24.24 |
| ATOM | 4631 | | | | 55.690 | -12.567 | 94.236 | 1.00 22.72 |
| ATOM | 4632 | | | | 55.485 | -11.549 | 95.322 | 1.00 25.26 |
| ATOM | 4633 | | 1 | | 54.235 | -10.977 | 95.535 | 1.00 23.80 |
| MOTA | 4634 | | | | 56.551 | -11.159 | 96.133 | 1.00 20.25 |
| ATOM | 4635 | | 4 | | 54.048 | -10.036 | 96.545 | 1.00 29.98 |
| ATOM | 4636 | | _ ^ ^ ^ | | 56.377 | -10.221 | 97.141 | |
| ATOM | 4637 | | | | 55.124 | | 97.350 | |
| ATOM | 4638 | | PHE B 204 | | 56.412 | -13.057 | 91.894 | |
| ATCM | 4639 | | PHE B 204 | | 55.613 | -13.540 | 91.091 | |
| ATOM | 4640 | | LEU B 205 | | | -13.449 | 91.986 | |
| ATOM | 4643 | | _ ^ ^ - | | | -14.472 | 2 91.114 | |
| ATOM | 1642 | | | , | 59.723 | -14.637 | 7 91.413 | 1.00 34.01 |
| ATOM | 164 | 3 CE | | | | | • | |
| | | | | | | | | |

| | | | CO 40E 11 | E 660 | 90.592 | 1.00 34.12 |
|------|------|---------------|--------------------|---------|--------|------------|
| MOTA | 4644 | CG LEU 3 205 | 60.495 -1 | | | 1.00 32.95 |
| MOTA | 4645 | CD1 LEU 3 205 | 60.356 -1 | | 89.109 | |
| | | CD2 LEU B 205 | 61.957 -1 | 5.629 | 91.005 | 1.00 36.49 |
| MOTA | 4646 | | 57.535 -1 | | 91.205 | 1.00 30.51 |
| ATOM | 4647 | | 57.467 -1 | 6 562 | 90.220 | 1.00 25.89 |
| ATOM | 4648 | O LEU B 205 | | | 92.382 | 1.00 30.43 |
| ATOM | 4649 | N GLU B 206 | 57.010 -1 | | | |
| | 4650 | CA GLU 3 206 | 56.338 -1 | 7.423 | 92.605 | |
| MOTA | | | 56.025 -1 | 7.601 | 94.093 | 1.00 34.77 |
| MOTA | 4651 | CD | 57.227 -1 | | 95.033 | 1.00 42.50 |
| ATOM | 4652 | | 57.718 -1 | | 95.270 | 1.00 45.76 |
| MOTA | 4653 | CD GLU 3 206 | | | 94.333 | 1.00 42.62 |
| ATOM | 4654 | OE1 GLU B 206 | 58.228 -1 | 5.438 | | 1.00 50.22 |
| | 4655 | OE2 GLU B 206 | 57.585 -1 | 5.602 | 96.413 | |
| MOTA | | C GLU B 206 | 55.045 -1 | 7.587 | 91.811 | 1.00 31.13 |
| ATOM | 4656 | 200 | 54.607 -1 | 8.708 | 91.563 | 1.00 28.18 |
| MOTA | 4657 | O GLU B 200 | 54.430 -1 | 6 472 | 91.425 | 1.00 25.16 |
| ATOM | 4658 | N GLU B 207 | 53.178 -1 | 6 499 | 90.664 | 1.00 28.78 |
| ATOM | 4659 | CA GLU B 207 | | | 90.695 | 1.00 30.76 |
| ATOM | 4660 | CB GLU B 207 | 52.546 -1 | | 90.093 | 1.00 29.39 |
| ATOM | 4661 | CG GLU B 207 | 52.121 -1 | | 92.093 | 1.00 27.87 |
| | 4662 | CD GLU B 207 | 52.057 <i>-</i> 1 | .3.151 | 92.230 | |
| MOTA | | OE1 GLU B 207 | 51.6 5 6 -1 | .2.477 | 91.261 | 1.00 24.38 |
| MOTA | 4663 | | 52.389 -1 | 2.636 | 93.316 | 1.00 25.36 |
| MOTA | 4664 | V | 53.453 -1 | 6.922 | 89.224 | 1.00 29.48 |
| MOTA | 4665 | C GLU B 207 | | | 88.351 | 1.00 27.48 |
| ATOM | 4666 | O GLU 3 207 | 53.658 -1 | | | 1.00 26.67 |
| ATOM | 4667 | N ILE B 208 | | 18.230 | 88.976 | 1.00 20.07 |
| | 4668 | CA ILE B 208 | 53.735 -1 | 18.754 | 87.646 | 1.00 32.60 |
| MOTA | | ^ ^ ^ | 54.789 -1 | 19.877 | 87.740 | 1.00 34.26 |
| MOTA | 4669 | | | 20.296 | 86.352 | 1.00 41.65 |
| MOTA | 4670 | CG2 ILE B 208 | | 19.404 | 88.532 | 1.00 36.07 |
| MOTA | 4671 | CG1 ILE B 208 | | 18.338 | 87.851 | 1.00 45.18 |
| ATOM | 4672 | CD1 ILE B 208 | | | 86.870 | 1.00 32.26 |
| ATOM | 4673 | C ILE B 208 | • | 19.289 | | |
| | 4674 | O ILE B 208 | | 19.799 | 85.759 | |
| ATOM | | N GLY B 209 | 51.328 - | 19.165 | 87.442 | 1.00 32.60 |
| MOTA | 4675 | | 50.139 - | 19.652 | 86.760 | 1.00 35.07 |
| ATOM | 4676 | | • • • • • • | 20.892 | 87.420 | 1.00 36.19 |
| ATOM | 4677 | C GLY B 209 | | 21.524 | 88.235 | 1.00 31.61 |
| MOTA | 4678 | O GLY B 209 | | | 87.066 | 1.00 36.98 |
| ATOM | 4679 | N GLU B 210 | | 21.245 | | 1.00 40.60 |
| ATOM | 4680 | CA GLU B 210 | | 22.412 | 87.647 | |
| | 4681 | CB GLU B 210 | | 21.964 | 88.672 | 1.00 37.98 |
| MOTA | | | 45.446 - | 21.234 | 88.058 | 1.00 42.78 |
| MOTA | 4682 | | 44.470 - | 20.717 | 89.098 | 1.00 48.41 |
| MOTA | 4683 | | 43.400 - | | 88.709 | 1.00 51.03 |
| MOTA | 4684 | OE1 GLU B 210 | | 20.814 | 90.306 | 1.00 49.90 |
| ATOM | 4685 | OE2 GLU B 210 | | | 86.564 | 1.00 39.48 |
| ATOM | 4686 | C GLU B 210 | 46.996 - | 23.248 | | |
| | 4687 | O GLU B 210 | 46.709 - | 22.751 | 85.471 | |
| ATOM | | N GLY B 211 | 46.736 - | 24.515 | 86.876 | 1.00 39.18 |
| ATOM | 4688 | | 46.087 - | 25.399 | 85.923 | 1.00 38.43 |
| MOTA | 1689 | | 46.877 - | 25.500 | 84.637 | 1.00 40.29 |
| MOTA | 4690 | C GLY B 211 | 48.101 - | 25 610 | 84.666 | 1.00 39.39 |
| ATOM | 4691 | O GLY B 211 | 40.101 | 25.010 | 83.504 | 1.00 40.90 |
| ATOM | 4692 | N LYS B 212 | 46.187 - | 25.458 | 82.219 | 1.00 43.53 |
| MOTA | 4693 | CA LYS B 212 | 46.864 - | -25.538 | | 1.00 43.33 |
| | 4694 | CB LYS B 212 | 45.842 - | 25.548 | 81.080 | 1.00 47.87 |
| ATOM | | | 44.795 - | 26.665 | 81.144 | 1.00 53.09 |
| ATOM | 4695 | 044 | 45.398 - | -28.076 | 81.130 | 1.00 58.61 |
| ATOM | 4696 | CD LYS 3 21 | 46.069 - | 28 454 | 82.452 | 1.00 59.78 |
| MOTA | 4697 | CE LYS B 21 | 46.009 | 20.434 | 82.420 | 1.00 62.17 |
| ATOM | 4698 | NZ LYS B 213 | 46.670 - | -23.023 | | |
| ATOM | 4699 | | 47.823 - | -24.363 | 82.040 | |
| | 4700 | | 48.797 - | -24.457 | 81.295 | |
| ATOM | | | 47.543 - | -23.262 | 82.731 | |
| MOTA | 4701 | | 48.384 - | -22.081 | 82.627 | 1.00 34.66 |
| ATOM | 4702 | | 49.625 | | 83.505 | 1.00 37.09 |
| ATOM | 4703 | C GLY B 21 | | 22.107 | 83.489 | |
| ATOM | 4704 | 0 GLY 3 21 | 50.425 | -21.100 | | |
| | 4705 | N LYS B 21 | 49.794 - | -23.180 | 84.273 | |
| ATOM | 4706 | | 50.953 | -23.297 | 85.148 | |
| MOTA | | | 50.886 · | -24.598 | 85.954 | 1.00 38.89 |
| ATOM | 1707 | | | -24.786 | 86.938 | 1.00 39.29 |
| ATOM | 4708 | G 515 B 41 | | -26 094 | 87.704 | 1.00 43.60 |
| ATCM | 1709 | CD LYS B 21 | 32.070 | 20.024 | • | |

| | 4710 | CE LYS B 214 | 53.04 | 7 -26.334 | 88.640 | 1.00 47.36 |
|------|------|---------------|---------|-------------|---------|------------|
| MOTA | 4710 | | 53 16 | 5 -25.264 | 89.666 | 1.00 54.03 |
| MOTA | 4711 | NZ LYS B 214 | | 9 -23.275 | 84.291 | 1.00 34.16 |
| ATOM | 4712 | C LYS B 214 | | | | |
| ATOM | 4713 | O LYS B 214 | 52.40 | | 83.438 | 1.00 34.70 |
| | 4714 | N GLY B 215 | 53.05 | 7 -22.279 | 84.523 | 1.00 33.58 |
| MOTA | | N GB1 B 215 | 54.27 | 5 -22.152 | 83.743 | 1.00 28.27 |
| MOTA | 4715 | CA GLY B 215 | | | 82.605 | 1.00 31.02 |
| ATOM | 4716 | C GLY B 215 | 54.10 | | | |
| | 4717 | O GLY B 215 | 55.03 | 3 -20.911 | 81.833 | 1.00 23.68 |
| MOTA | | N TYR B 216 | 52.91 | 8 -20.564 | 82.493 | 1.00 22.45 |
| MOTA | 4718 | N 11K B 210 | 52.68 | | 81.426 | 1.00 24.03 |
| ATOM | 4719 | CA TYR B 216 | | | 80.603 | 1.00 17.60 |
| ATOM | 4720 | CB TYR B 216 | 51.45 | | | 1.00 25.96 |
| MOTA | 4721 | CG TYR B 216 | . 51.68 | 32 -21.291 | 79.806 | |
| | 4722 | CD1 TYR B 216 | 51.69 | 2 -22.538 | 80.435 | 1.00 21.41 |
| ATOM | | | 51 98 | 3823 .704 | 79.729 | 1.00 23.78 |
| ATOM | 4723 | | 51.97 | | 78.439 | 1.00 19.62 |
| MOTA | 4724 | CD2 TYR B 216 | 21.2 | | 77.72-2 | 1.00 26.39 |
| ATOM | 4725 | CE2 TYR B 216 | | 59 -22.402 | | |
| | 4726 | CZ TYR B 216 | 52.27 | 77 -23.630 | 78.379 | 1.00 29.35 |
| MOTA | | OH TYR B 216 | 52.5 | 77 -24.782 | 77.690 | 1.00 27.75 |
| ATOM | 4727 | | 52.5 | | 81.884 | 1.00 24.53 |
| ATOM | 4728 | C TYR B 216 | | | 81.159 | 1.00 18.99 |
| ATOM | 4729 | O TYR B 216 | 52.0 | | | 1.00 21.41 |
| MOTA | 4730 | N ASN B 217 | 53.0 | | 83.098 | |
| | 4731 | CA ASN B 217 | 53.0 | 73 -16.534 | 83.642 | 1.00 21.23 |
| MOTA | | | 51.9 | | 84.669 | 1.00 16.78 |
| MOTA | 4732 | | 51.8 | | 85.162 | 1.00 22.07 |
| MOTA | 4733 | CG ASN B 217 | | | 86.163 | 1.00 23.13 |
| ATOM | 4734 | OD1 ASN B 217 | 52.5 | | | 1.00 19.26 |
| ATOM | 4735 | ND2 ASN B 217 | | 46 -14.058 | 84.435 | • • |
| | 4736 | C ASN B 217 | 54.4 | 37 -16.339 | 84.291 | 1.00 19.40 |
| MOTA | | | | 57 -17.145 | 85.124 | 1.00 19.28 |
| MOTA | 4737 | 010 | 55.0 | 30 -15.273 | 83.905 | 1.00 18.65 |
| ATOM | 4738 | N LEU B 218 | 55.1 | 50 -15.275 | 84.444 | 1.00 16.41 |
| MOTA | 4739 | CA LEU B 218 | 56.4 | 59 -15.004 | | |
| ATOM | 4740 | CB LEU B 218 | 57.5 | 12 -15.244 | 83.368 | 1.00 18.29 |
| | | CG LEU B 218 | 58.8 | 51 -15.872 | 83.782 | 1.00 28.15 |
| MOTA | 4741 | | 59 B | 73 -15.563 | 82.695 | 1.00 20.50 |
| MOTA | 4742 | V | 50.3 | 32 -15.348 | 85.116 | 1.00 22.53 |
| MOTA | 4743 | CD2 LEU B 218 | | | 84.926 | 1.00 17.89 |
| ATOM | 4744 | C LEU B 218 | 56.5 | | | |
| ATOM | 4745 | O LEU B 218 | 56.4 | 69 -12.627 | 84.128 | 1.00 14.48 |
| | | | 56.8 | 59 -13.395 | 86.219 | 1.00 14.09 |
| ATOM | 4746 | N ASN B 219 | | 44 -12.075 | 86.821 | 1.00 18.41 |
| ATOM | 4747 | CA ASN B 219 | | 38 -11.922 | 88.111 | 1.00 14.64 |
| ATOM | 4748 | CB ASN B 219 | | | 87.868 | 1.00 27.12 |
| ATOM | 4749 | CG ASN B 219 | 54.7 | 48 -11.898 | | |
| | 4750 | OD1 ASN B 219 | 54.2 | 86 -11.332 | 86.880 | 1.00 20.21 |
| ATOM | | ND2 ASN B 219 | 53.9 | 82 -12.480 | 88.787 | 1.00 23.62 |
| MOTA | 4751 | | 58 5 | 04 -11.843 | 87.172 | 1.00 20.39 |
| MOTA | 4752 | C ASN B 219 | 50.5 | 15 -12.672 | 87.841 | 1.00 20.41 |
| ATOM | 4753 | O ASN B 219 | 29.1 | 15 -12.072 | | 1.00 15.11 |
| MOTA | 4754 | N ILE B 220 | 59.0 | 56 -10.717 | 86.729 | |
| ATOM | 4755 | CA ILE B22C | 60.4 | 41 -10.394 | 87.033 | 1.00 17.16 |
| | | CB ILE B 220 | 61.2 | 50 -10.083 | 85.740 | 1.00 20.78 |
| ATOM | 4756 | CB 1DB D 220 | 62.7 | | 86.094 | 1.00 18.08 |
| MOTA | 4757 | CG2 ILE B 22C | 62.7 | .38 -11.250 | | 1.00 17.62 |
| ATOM | 4758 | CG1 ILE B 220 | 61.1 | .36 -11.230 | 05.730 | 1.00 20.72 |
| ATOM | 4759 | CD1 ILE B 220 | 61.6 | 46 -12.590 | 85.273 | 1 00 20 17 |
| | 4760 | C ILE B 220 | 60.4 | 75 -9.161 | | 1.00 21.17 |
| MOTA | | | 60.5 | 65 -8.036 | 87.470 | 1.00 16.03 |
| MOTA | 4761 | | 60.3 | | | 1.00 21.74 |
| ATOM | 4762 | N PRO B 221 | 60.5 | 35 -10.619 | | 1.00 22.96 |
| ATOM | 4763 | CD PRO B 221 | | | | 1.00 19.16 |
| ATOM | 4764 | CA PRO B 221 | 60.3 | | | 1.00 19.10 |
| | 4765 | CB PRO B 221 | 59.9 | | | 1.00 19.40 |
| ATOM | | | | 64 -10.251 | 91.407 | 1.00 23.02 |
| ATOM | 4766 | | 61.7 | | | 1.00 22.42 |
| ATOM | 4767 | C PRO B 221 | | | | 1.00 20.71 |
| ATOM | 4768 | O PRO B 221 | 62. | 780 -8.369 | | 1.00 22.74 |
| | 4769 | N LEU B 222 | 61.8 | | | 1.00 22.79 |
| ATOM | | CA LEU B 222 | 63. | | | 1.00 21.18 |
| ATOM | 4770 | | 63.4 | _ | | 1.00 17.21 |
| MOTA | 4771 | | 63.4 | | | 1.00 20.26 |
| ATCM | 4772 | CG LEU B 222 | | | | 1.00 20.00 |
| ATOM | 4773 | CD1 LEU B 222 | 63.4 | | | 1.00 21.93 |
| | 4774 | CD2 LEU B 222 | 64. | | | 1.00 20 00 |
| ATCM | 4775 | | 63. | 335 -4.616 | 91.353 | 1.00 20.04 |
| ATOM | 4/13 | | | | • | |

| | | | | | | | 4 00 17 50 |
|--------|-------------|-------------------|---------|-----------------|--------|--------|------------|
| | 4776 | O LEU B | 222 | 62.350 | | 91.806 | 1.00 17.58 |
| ATOM | - | | | 64.571 | -4.394 | 91.830 | 1.00 19.48 |
| ATOM | 4777 | | 223 | 65.806 | -5.072 | 91.400 | 1.00 16.80 |
| MOTA | 4778 | CD PRO B | 223 | | | 92.915 | 1.00 20.38 |
| MOTA | 4779 | CA PRO B | 223 | 64.873 | -3.454 | - | |
| | 4780 | | 223 | 66.274 | -3.881 | 93.327 | |
| ATOM | | | | 66.884 | -4.161 | 91.973 | 1.00 19.74 |
| ATOM | 4781 | CG PRO B | 223 | | -1.971 | 92.553 | 1.00 21.39 |
| ·ATOM | 4782 | C PRO B | 223 | 64.818 | | | 1.00 17.16 |
| ATOM | 4783 | C PRO B | 223 | 64.815 | -1.598 | 91.380 | |
| | 4784 | N LYS B | 224 | 64.798 | -1.142 | 93.589 | 1.00 20.65 |
| MOTA | | | 224 | 64.755 | 0.311 | 93.462 | 1.00 27.00 |
| MOTA | 4785 | CA. LYS B | 224 | | 0.938 | 94.844 | 1.00 36:47 |
| MOTA | 4786 | CB LYS B | 224 | 64.577 | | | 1.00 37.72 |
| ATOM | 4787 | CG LYS B | 224 | 63.415 | 0.389 | 95651 | |
| • | 4788 | CD LYS B | 224 | 63.541 | 0.833 | 97.101 | 1.00 42.06 |
| ATOM | | | | 62.420 | 0.276 | 97.955 | 1.00 45.18 |
| ATOM | 4789 | | | 62.645 | | 99.399 | 1.00 46.30 |
| ATOM | 4790 | | 224 | | | 92.874 | 1.00 27.01 |
| MOTA | 4791 | C LYS B | 224 | 66.071 | 0.808 | 92.074 | |
| | 4792 | O LYS B | 224 | 67.098 | 0.139 | 92.995 | |
| ATOM | | | 225 | 66.038 | 1.989 | 92.259 | 1.00 22.66 |
| MOTA | 1793 | | 225 | 67.239 | 2.565 | 91.669 | 1.00 25.67 |
| MOTA | 4794 | | | | 1.809 | 90.459 | 1.00 24.95 |
| MOTA | 4795 | | 225 | 67.768 | | | 1.00 26.83 |
| MOTA | 4796 | O GLY B | 225 | 68.917 | 1.975 | 90.069 | 1.00 20.00 |
| | 4797 | N LEU B | 226 | 6 6 .926 | 0.980 | 89.855 | 1.00 21.79 |
| ATOM | | | 226 | 67.319 | 0.180 | 88.692 | 1.00 22.31 |
| ATOM | 4798 | | | 66.067 | -0.473 | 88.099 | 1.00 23.29 |
| ATOM | 1799 | | 226 | | | 87.091 | 1.00 26.71 |
| ATOM | 4800 | CG LEU B | 226 | 66.238 | -1.605 | | 1.00 25.44 |
| ATOM | 4801 | CD1 LEU B | 226 | 66.846 | -2.804 | 87.813 | |
| | | CD2 LEU B | 226 | 64.877 | -1.997 | 86.508 | 1.00 22.96 |
| MOTA | 4802 | | 226 | 68.008 | 1.017 | 87.603 | 1.00 22.66 |
| MOTA | 4803 | | | 67.517 | 2.087 | 87.250 | 1.00 20.19 |
| ATOM | 4804 | | 226 | | | 87.060 | 1.00 15.52 |
| ATOM | 4805 | n ASN B | 227 | 69.134 | 0.549 | | |
| | 4806 | CA ASN B | 227 | 69.794 | 1.317 | 85.998 | |
| ATOM | | | 227 | 71.304 | 1.474 | 86.270 | 1.00 20.43 |
| ATOM | 4807 | | | 72.062 | 0.161 | 86.206 | 1.00 28.97 |
| ATOM | 4808 | | 227 | | -0.546 | 85.199 | 1.00 24.30 |
| ATOM | 4809 | | 227 | 72.015 | | 87.276 | 1.00 20.88 |
| MOTA | 4810 | ND2 ASN B | 227 | 72.786 | -0.160 | | 1.00 21.26 |
| | 4811 | C ASN B | 227 | 69.548 | 0.671 | 84.630 | |
| ATOM | | | 227 | 69.004 | -0.432 | 84.555 | 1.00 18.90 |
| ATOM | 4812 | | | 69.949 | 1.347 | 83.552 | 1.00 20.98 |
| ATOM | 4813 | N ASP B | 220 | 69.720 | 0.817 | 82.208 | 1.00 22.51 |
| MOTA | 4814 | CA ASP B | 228 | | | 31.126 | 1.00 23.46 |
| ATOM | 4815 | CB ASP B | 228 | 70.270 | 1.753 | | 1.00 26.12 |
| | 4816 | CG ASP 3 | 228 | 69.596 | 3.113 | 81.119 | |
| MOTA | | OD1 ASP B | | 68.387 | 3.193 | 81.415 | 1.00 26.75 |
| ATCM | 4817 | ODI ASE D | 228 | 70.276 | 4.101 | 80.773 | 1.00 30.22 |
| atom | 4818 | OD2 ASP B | 220 | 70.286 | -0.573 | 81.952 | 1.00 23.49 |
| ATOM | 4819 | C ASP B | 228 | | | 81.288 | 1.00 19.31 |
| ATOM | 4820 | O ASP B | 228 | 69.651 | -1.390 | | 1.00 22.24 |
| ATCM | 4821 | N ASN B | | 71.484 | -0.836 | 82.453 | 1.00 22.24 |
| | | - · · · · · - · - | 229 | 72.111 | -2.135 | 82.250 | 1.00 23.30 |
| ATOM | 4822 | CA ASN B | 220 | 73.562 | -2.101 | 82.737 | 1.00 20.99 |
| ATOM | 4823 | CB ASN B | 223 | | | 81.859 | 1.00 25.71 |
| ATCM | 4824 | CG ASN B | 229 | 74.441 | | | 1.00 26.40 |
| ATOM | 4825 | OD1 ASN B | 229 | 74.644 | -1.538 | 80.678 | 1.00 20.10 |
| | 4826 | ND2 ASN B | 229 | 74.955 | | 82.417 | 1.00 27.44 |
| ATOM | | | 229 | 71.341 | | 82.943 | 1.00 23.74 |
| atom | 4827 | C ASN B | 220 | 71.207 | | 82.402 | 1.00 20.51 |
| ATCM | ∔828 | C ASN B | 229 | | | 84.139 | |
| MOTA | 4829 | N GLU B | 230 | 70.832 | | | |
| ATOM | 4830 | | 230 | 70.069 | | 84.874 | |
| | | | 230 | 69.799 | -3.480 | 86.297 | |
| ATOM | 4831 | CD GLU 2 | 230 | 71.069 | -3.201 | 87.087 | 1.00 27.28 |
| MOTA | 4832 | | 230 | | | 88.470 | 1.00 27.47 |
| ATOM | 4833 | CD GLU B | ن کے ک | 70.792 | | | |
| ATOM | 4834 | OE1 GLU E | 3 230 | 70.086 | | | |
| | 4835 | | 230 | 71.286 | -3.232 | 89.455 | |
| ATOM | | | 2 730 | 68.749 | | 84.146 | 1.00 24.25 |
| ATOM | 4836 | | 220 | 68.347 | | | 1.00 15.89 |
| ATCM | 4837 | O GLU E | 0 د د | | | | |
| ATOM | ;838 | N PHE | 3 231 | 68.391 | -3.242 | | |
| | 4839 | | 3 231 | 66.814 | | | 1.00 22.04 |
| ATOM | | | 3 231 | 66.210 | -2.079 | 82.529 | |
| , ATOM | 4840 | | 2 2 2 1 | 64.803 | | | 1.00 26.13 |
| ATOM | 4841 | . CG PHE E | 221 | 54.505 | | • | |

| | 4042 | CD1 | PHE B | 231 | 63.738 | -2.514 | 82.805 | 1.00 25.00 |
|--------------|--------------|----------|-------|-------|------------------|--------------------|------------------|--------------------------|
| MOTA | 4842 | | PHE B | 231 | 64.550 | -1.956 | 80.627 | 1.00 22.93 |
| MOTA | 4843 | | PHE B | | 62.440 | -2.618 | 82.304 | 1.00 25.03 |
| MOTA | 4844 | | PHE B | | 63.250 | -2.059 | 80.114 | 1.00 27.46 |
| ATOM | 4845 | | PHE B | | 62.196 | -2.390 | 80.957 | 1.00 20.25 |
| MOTA | 4846 | CZ | PHE B | | 66.978 | -4.288 | 81.677 | 1.00 23.14 |
| ATOM | 4847 | C | | | 66.221 | -5.239 | 81.464 | 1.00 20.02 |
| MOTA | 4848 | 0 | PHE B | | 67.963 | -3.952 | 80.845 | 1.00 22.02 |
| ATOM | 4849 | N | LEU B | 222 | 68.200 | -4.697 | 79.614 | 1.00 19.97 |
| MOTA | 4850 | CA | LEU B | | 69.192 | -3.942 | 78.734 | 1.00 24.99 |
| MOTA | 4851 | CB | LEU B | | 68.665 | -2.581 | 78.263 | 1.00 29.73 |
| MOTA | 4852 | CG | LEU B | | 69.746 | -1.856 | 77.454 | 1.00 28.11 |
| | 4853 | CDI | LEU B | 232 | 67.409 | -2.784 | 77.414 | 1.00 26.54 |
| MOTA | 4854 | | LEU B | | 68.688 | -6.119 | 79.898 | 1.00 19.25 |
| MOTA | 4855 | C | LEU B | | 68.365 | -7.051 | 79,162 | 1.00 19.49 |
| ATOM | 4856 | 0 | PHE B | 223 | 69.468 | -6.280 | 80.962 | 1.00 20.50 |
| ATOM | 4857 | N | PHE B | 222 | 69.950 | -7.599 | 81.378 | 1.00 20.70 |
| ATOM | 4858 | CA | PHE E | | 70.825 | -7.471 | 82.632 | 1.00 23.75 |
| MOTA | 4859 | CB CG | PHE E | | 71.217 | -8.790 | 83.239 | 1.00 28.58 |
| MOTA | 4860 | | PHE E | | 72.285 | -9.519 | 82.731 | 1.00 30.48 |
| ATOM | 4861 | CD2 | PHE E | | 70.481 | -9.328 | 84.294 | 1.00 25.32 |
| MOTA | 4862 | CE1 | PHE E | | 72.617 | -10.762 | 83.262 | 1.00 31.87 |
| MOTA | 4863 | | PHE E | | 70.803 | -10.573 | 84.832 | 1.00 31.26 |
| ATOM | 4864 | CZ | PHE E | 233 | 71.871 | -11.292 | 84.317 | 1.00 32.29 |
| ATOM | 4865 4866 | | PHE | | 68.712 | -8.439 | 81.727 | 1.00 20.23 |
| ATOM | 4867 | 0 | PHE E | | 68.553 | -9.567 | 81.270 | 1.00 21.56 |
| MOTA | 4868 | N | ALA E | | 67.842 | -7.878 | 82.560 | 1.00 21.26 |
| MOTA | 4869 | CA | ALA E | | 66.626 | -8.576 | 82.963 | 1.00 19.60 |
| MOTA | 4870 | CB | ALA I | | 65.835 | -7.733 | 83.950 | 1.00 19.25 |
| MOTA | 4871 | c | ALA I | | 65.772 | -8.898 | 81.749 | 1.00 18.87 |
| MOTA MOTA | 4872 | ō | ALA I | | 65.253 | -10.010 | 81.624 | 1.00 21.91 |
| ATOM | 4873 | N | LEU I | | 65.634 | -7.934 | 80.845 | 1.00 20.29 |
| ATOM | 4874 | CA | LEU I | | 64.822 | -8.141 | 79.652 | 1.00 19.53 |
| ATOM | 4875 | CB | LEU I | | 64.773 | -6:874 | 78.795 | 1.00 24.07 |
| ATOM | 4876 | ÇG | | 3 235 | 63.465 | -6.607 | 78.024 | 1.00 27.87 |
| MOTA | 4877 | CD1 | LEU I | 3 235 | 63.783 | -5.813 | 76.770 | 1.00 20.77 |
| ATOM | 4878 | CD2 | LEU ! | 3 235 | 62.761 | -7.897 | 77.664 | 1.00 26.94 1.00 20.79 |
| ATOM | 4879 | С | | 3 235 | 65.376 | -9.276 | 78.795 | '_ |
| MOTA | 4880 | 0 | | B 235 | 64.648 | -10.205 | 78.431 | 1.00 18.25 1.00 19.33 |
| ATOM | 4881 | N | GLU : | B 236 | 66.665 | -9.191 | 78.462 | 1.00 19.33 |
| MOTA | 4882 | CA | GLU : | в 236 | 67.303 | | 77.629 77.384 | 1.00 27.33 |
| ATOM | 4883 | CB | | В 236 | 68.777 | -9.853 | 76.548 | 1.00 43.60 |
| MOTA | 4884 | CG | GLU | | 68.969 | -8.597 | 76.259 | 1.00 45.19 |
| MOTA | 4885 | CD | GLU | | 70.428 | -8.292 | 75.538 | 1.00 48.77 |
| ATOM | 4886 | OEl | | | 70.697 | -7.309 | 76.751 | 1.00 52.72 |
| ATOM | 4887. | OE2 | GLU | B 236 | 71.300 | -9.032 | 78.209 | 1.00 24.89 |
| MOTA | 4888 | С | GLU | B 236 | 67.20. | -11.607 -12.552 | 77.501 | 1.00 22.06 |
| ATCM | 1889 | 0 | GLU | B 236 | 66.865 | -11.748 | 79.492 | 1.00 24.20 |
| ATCM | 4890 | N | LYS | B 237 | 67.520 | | 80.130 | 1.00 27.10 |
| MOTA | 4891 | CA | | B 237 | | -12.984 | 81.562 | |
| ATOM | 4892 | СВ | LYS | B 237 | | -12.641 | 81.650 | 1.00 29.46 |
| ATOM | 4893 | CG | LYS | B 237 | 70 305 | -13.683 | 80.924 | 1.00 31.65 |
| ATOM | 4894 | CD | LYS | B 237 | 70.303 | -13.356 | 80.993 | 1.00 39.70 |
| MOTA | 4895 | CE | LYS | B 237 | 72.702 | -14.363 | 80.242 | 1.00 46.74 |
| MOTA | 4896 | NZ | LYS | B 237 | 72.300 66 010 | -13.615 | 80.143 | 1.00 30.92 |
| ATOM | 4897 | C | LYS | B 237 | 65.017 | -14.766 | 79.763 | 1.00 31.42 |
| MOTA | 4898 | 0 | LYS | B 237 | | -12.806 | 80.573 | 1.00 25.86 |
| MOTA | 4899 | Ŋ | SER | B 238 | 63.037 | -13.280 | 80.620 | 1.00 27.98 |
| ATOM | 4900 | CA | SER | B 238 | | -12.241 | 81.289 | 1.00 23.89 |
| MOTA | 1901 | CB | SER | B 238 | 62.110 | -11.028 | | 1.00 29.27 |
| ATCM | 1902 | OG | SER | B 238 | 52.730 | -13.642 | 79.229 | 1.00 28.32 |
| ATOM | 4903 | C | SER | B 238 | 62 187 | -14.605 | | 1.00 29.65 |
| MOTA | 1904 | 0 | SER | B 238 | 63 536 | -12.886 | | 1.00 27.39 |
| ATOM | 4905 | N | LEU | B 239 | 63.550 | -13.192 | | 1.00 32.52 |
| ATCM | 4906 | | LEU | B 239 | | -12.129 | | |
| ATOM | 4907 | CB | LEU | в 239 | 099 | | • | |

| | | CG LEU B 239 | 62.833 | -10.772 | 75.895 | 1.00 36.06 |
|--------|------|---------------|--------|----------|--------|------------|
| MOTA | 4908 | | 63.404 | -9.836 | 74.842 | 1.00 29.64 |
| ATOM | 4909 | CD1 LEU B 239 | | | 75.667 | 1.00 30.73 |
| MOTA | 4910 | CD2 LEU B 239 | 61.338 | | | |
| ATOM | 4911 | C LEU B 239 | 63.598 | -14.563 | 76.430 | 1.00 34.15 |
| | 4912 | O LEU B 239 | 62.879 | -15.340 | 75.803 | 1.00 33.23 |
| ATOM | | | 64.844 | -14.859 | 76.788 | 1.00 31.39 |
| MOTA | 4913 | 0.40 | | -16.152 | 76.472 | 1.00 33.79 |
| MOTA | 4914 | | 66.859 | | 77.011 | 1.00 38.51 |
| ATOM | 4915 | CB GLU B 240 | | | | 1.00 40.56 |
| ATOM | 4916 | CG GLU B. 240 | 67.878 | | 76.275 | |
| ATOM | 4917 | CD GLU B 240 | 69.256 | -15.532 | 76.903 | 1.00 48.20 |
| | 4918 | CE1 GLU B 240 | 69.685 | -16.679 | 77.161 | 1.00 45.36 |
| MOTA | | | 69.912 | | 77.130 | 1.00 48.21 |
| MOTA | 4919 | | 64.604 | | 77.108 | 1.00 33.23 |
| ATOM | 4920 | C GLU B 240 | 64.391 | | 76.510 | 1.00 32.15 |
| MOTA | 4921 | O GLU B 240 | 64.391 | -10.310 | 78.331 | 1.00 29.72 |
| ATOM | 4922 | N ILE B 241 | 64.146 | -17.017 | | 1.00 29.85 |
| ATOM | 4923 | CA ILE B 241 | | -17.989 | 79.047 | |
| ATOM | 4924 | CB ILE B 241 | 63.006 | -17.489 | 80.466 | 1.00 30.42 |
| | 4925 | CG2 ILE B 241 | | -18.456 | 81.162 | 1.00 29.88 |
| MOTA | | | 64.309 | -17.311 | 81.254 | 1.00 29.77 |
| ATOM | 4926 | | | -16.760 | 82.654 | 1.00 32.92 |
| ATOM | 4927 | | | -18.247 | 78.298 | 1.00 34.65 |
| ATOM | 4928 | C ILE B 241 | | | 78.149 | 1.00 30.22 |
| ATOM | 4929 | C ILE B 241 | 61.592 | -19.396 | | 1.00 31.16 |
| ATOM | 4930 | N VAL B 242 | 61.379 | -17.178 | 77.823 | |
| ATOM | 4931 | CA VAL B 242 | | -17.312 | 77.105 | 1.00 34.55 |
| | 4932 | CB VAL B 242 | 59.476 | -15.937 | 76.825 | 1.00 30.77 |
| MOTA | | | 58.191 | -16.113 | 76.038 | 1.00 32.18 |
| ATOM | 4933 | | | -15.214 | 78.140 | 1.00 31.57 |
| ATOM | 4934 | | | -18.042 | 75.787 | 1.00 36.56 |
| ATOM | 4935 | c VAL B 242 | | | 75.453 | 1.00 33.93 |
| ATOM | 4936 | O VAL B 242 | | -18.959 | | 1.00 38.64 |
| MOTA | 4937 | N LYS B 243 | | -17.527 | 75.042 | 1.00 44.36 |
| ATOM | 4938 | CA LYS B 243 | 61.659 | -18.241 | 73.760 | 1.00 44.30 |
| | 4939 | CB LYS B 243 | 62.966 | -17.659 | 73.214 | 1.00 48.33 |
| ATOM | 4940 | CG LYS B 243 | 62.810 | -16.399 | 72.386 | 1.00 53.88 |
| MOTA | | | 62.185 | -16.718 | 71.036 | 1.00 53.72 |
| MOTA | 4941 | CD LYS B 243 | | -17.681 | 70.242 | 1.00 54.69 |
| MOTA | 4942 | CE LYS B 243 | | -18.025 | 68.923 | 1.00 57.75 |
| . ATOM | 4943 | NZ LYS B 243 | 62.430 | 10.025 | 73.824 | 1.00 43.21 |
| MOTA | 4944 | C LYS B 243 | 61.793 | -19.755 | | 1.00 42.92 |
| ATOM | 4945 | O LYS B 243 | | -20.455 | 72.884 | |
| ATOM | 4946 | : GLU B 244 | | -20.257 | 74.935 | |
| | 4947 | CA GLU B 244 | | -21.687 | 75.085 | 1.00 47.72 |
| MOTA | 4948 | CB GLU B 244 | 63.669 | -21.925 | 76.075 | 1.00 50.89 |
| MOTA | | | 64.080 | -23.378 | 76.208 | 1.00 57.16 |
| MOTA | 4949 | | | -23.564 | 77.173 | 1.00 57.74 |
| MOTA | 4950 | CD GLU B 244 | | -22.967 | 76.942 | 1.00 60.18 |
| ATOM | 4951 | CE1 GLU B 244 | | | 78.160 | 1.00 61.59 |
| ATOM | 4952 | OE2 GLU B 244 | | -24.308 | | 1.00 47.78 |
| ATOM | 4953 | C GLU B 244 | 61.312 | -22.507 | 75.505 | |
| MOTA | 4954 | O GLU B 244 | 61.376 | -23.736 | 75.544 | 1.00 51.39 |
| | 4955 | N VAL B 245 | 60.200 | -21.851 | 75.805 | 1.00 43.31 |
| MOTA | | CA VAL B 245 | 59.019 | -22.589 | 76.230 | 1.00 43.55 |
| ATOM | 4956 | | 58 867 | -22.514 | 77.771 | 1.00 45.89 |
| ATOM | 4957 | | 57 665 | -23.322 | 78.231 | 1.00 49.90 |
| ATOM | 4958 | CG1 VAL B 245 | 57.005 | -23.040 | 78.435 | 1.00 46.37 |
| ATOM | 4959 | CG2 VAL B 245 | 00.737 | 22.090 | 75.565 | 1.00 41.01 |
| ATOM | 4960 | C VAL B 245 | 57.727 | -22.115 | | 1.00 39.36 |
| MOTA | 4961 | O VAL B 245 | 56.659 | -22.676 | 75.798 | 1.00 34.37 |
| | 4962 | ☐ PHE B 246 | 57.814 | -21.101 | 74.716 | 1.00 34.37 |
| MOTA | | CA PHE B 246 | 56,610 | -20.602 | 74.077 | 1.00 34.36 |
| MOTA | 4963 | | 55.986 | -19.517 | 74.958 | 1.00 30.80 |
| MOTA | 4964 | | | -19.230 | 74.644 | 1.00 32.57 |
| MOTA | 4965 | CG PHE B 246 | 52 5/0 | -20.142 | 74.989 | 1.00 27.72 |
| MOTA | 4966 | CD1 PHE B 246 | 53.340 | 10 040 | | 1.00 28.20 |
| ATOM | 4967 | CD2 PHE B 246 | 54.174 | -18.048 | | |
| ATOM | 4968 | CE1 PHE B 246 | | -19.878 | | |
| | 4969 | | | -17.773 | | |
| ATOM | | 246 | | -18.689 | | 1.00 26.18 |
| ATOM | 1970 | | | -20.040 | 72.682 | |
| MOTA | 1971 | | | -19.153 | | 1.00 31.73 |
| ATOM. | 4972 | 0.47 | | -20.568 | | 00 |
| ATOM | 4973 | : GLU B 247 | 50.20 | . 20.500 | • | |

| | 4074 | C D | GLU B | 247 | 56.3 | 363 | -20.137 | 70.296 | 1.00 40.73 |
|------|------|-----|-------|------------|------|-------|---------|--------|------------|
| ATOM | 4974 | | | | | | -21.347 | 69.370 | 1.00 43.38 |
| ATOM | 4975 | | GLU B | | | | -22.702 | 70.073 | 1.00 51.49 |
| MOTA | 4976 | | GLU B | | | | -23.214 | 70.718 | 1.00 55.29 |
| MOTA | 4977 | | GLU B | | | | | | 1.00 49.08 |
| ATOM | 4978 | | GLU B | | | | -22.601 | 71.691 | |
| ATOM | 4979 | OE2 | GLU B | 247 | | | -24.246 | 70.241 | 1.00 60.95 |
| MOTA | 4980 | С | GLU B | 247 | | | -19.379 | 69.939 | 1.00 39.04 |
| | 4981 | ō | GLU B | 247 | 54. | 129 | -19.960 | 69.436 | 1.00 39.49 |
| MOTA | | | PRO B | | | | -18.064 | 70.182 | 1.00 35.13 |
| MOTA | 4982 | N | PRO B | | | | -17.279 | 70.733 | 1.00 33.57 |
| ATOM | 4983 | CD | | | | | -17.188 | 69.916 | 1.00 36.03 |
| ATOM | 4984 | CY | PRO B | | | | -15.878 | 70.562 | 1.00 35.33 |
| MOTA | 4985 | CB | PRO B | | | | | 70.332 | 1.00 32.85 |
| MOTA | 4986 | CG | PRO B | | | | -15.880 | | 1.00 32.03 |
| MOTA | 4987 | C | PRO B | 248 | 53. | 563 | -16.990 | 68.457 | |
| ATOM | 4988 | 0 | | 248 | | | -16.808 | 67.604 | 1.00 29.38 |
| ATOM | 4989 | N | GLU B | 249 | 52. | 263 | -17.012 | 68.182 | 1.00 32.23 |
| | 4990 | CA | | 249 | 51. | 773 | -16.782 | 66.828 | 1.00 29.35 |
| MOTA | 4991 | CB | GLU B | 249 | 50. | 374 | -17.366 | 66.645 | 1.00 31.87 |
| MOTA | | CG | GLU B | 249 | | | -18.867 | 66.787 | 1.00 28.64 |
| ATOM | 4992 | | GLU B | 249 | | | -19.338 | 66.747 | 1.00 33.37 |
| MOTA | 4993 | CD | | 249 | | | -18.917 | 67.630 | 1.00 26.38 |
| ATOM | 4994 | | | | | | -20.115 | 65.835 | 1.00 37.71 |
| MOTA | 4995 | | | 249 | | | -15.273 | 66.650 | 1.00 28.25 |
| ATOM | 4996 | С | GLU B | 249 | | | | 65.537 | 1.00 21.47 |
| MOTA | 4997 | 0 | GLU B | 249 | | | -14.765 | 67.768 | 1.00 21.77 |
| MOTA | 4998 | N | VAL B | 250 | | | -14.564 | | 1.00 21.41 |
| ATOM | 4999 | CA | VAL B | 250 | | 459 | | 67.756 | 1.00 21.41 |
| ATOM | 5000 | CB | VAL B | 250 | | | -12.676 | 67.357 | |
| ATOM | 5001 | CG1 | VAL B | 250 | | 037 | | 68.378 | 1.00 20.96 |
| ATOM | 5002 | CG2 | VAL B | 250 | | 931 | | 67.243 | 1.00 24.68 |
| ATOM | 5003 | С | VAL B | | | | -12.608 | 69.168 | 1.00 22.88 |
| | 5004 | Ö | VAL B | 250 | 51. | 592 | -13.354 | 70.133 | 1.00 18.00 |
| MOTA | 5005 | N | TYR B | | 52. | 201 | -11.359 | 69.295 | 1.00 20.28 |
| MOTA | | CA | TYR B | 251 | 52. | 481 | -10.823 | 70.620 | 1.00 22.33 |
| MOTA | 5006 | | TYR B | 251 | | 956 | -11.043 | 70.999 | 1.00 20.67 |
| MOTA | 5007 | ĊВ | TYR B | 251 | | | -10.045 | 70.427 | 1.00 21.89 |
| MOTA | 5008 | CG | TIRD | 751 751 | | 198 | -8.834 | 71.072 | 1.00 19.31 |
| MOTA | 5009 | CD1 | TYR B | | | 129 | -7.922 | 70.562 | 1.00 23.73 |
| MOTA | 5010 | CE1 | | 251 | | 651 | | 69.254 | 1.00 18.72 |
| MOTA | 5011 | CD2 | | | | | -9.417 | 68.734 | 1.00 22.71 |
| MOTA | 5012 | CE2 | TYR B | 251 | | 580 | | 69.390 | 1.00 27.33 |
| MOTA | 5013 | CŻ | TYR B | 251 | | 813 | -8.220 | | 1.00 23.18 |
| MOTA | 5014 | oh | TYR B | 251 | | .705 | -7.308 | 68.865 | 1.00 25.71 |
| ATOM | 5015 | C | TYR B | 251 | | .134 | -9.349 | 70.732 | 1.00 20.14 |
| MOTA | 5016 | 0 | TYR B | 251 | | . 095 | -8.622 | 69.728 | |
| ATOM | 5017 | N | LEU B | 252 | | . 834 | -8.930 | 71.958 | 1.00 21.13 |
| ATOM | 5018 | CA | LEU B | 252 | 51 | . 533 | -7.532 | 72.252 | 1.00 24.61 |
| MOTA | 5019 | СВ | LEU B | 252 | 50 | . 154 | -7.373 | 77.897 | 1.00 22.88 |
| | 5020 | CG | LEU B | 252 | 48 | .915 | -7.435 | ¹1.996 | 1.00 23.73 |
| MOTA | 5021 | CDI | LEU B | 252 | 48 | .779 | | 1.360 | 1.00 23.18 |
| ATOM | | CD2 | | 252 | | . 697 | | 72.833 | 1.00 29.06 |
| ATOM | 5022 | | LEU B | 252 | | .610 | | 73.217 | 1.00 24.77 |
| ATOM | 5023 | C | LEU D | 252 | | .064 | | 74.076 | |
| MOTA | 5024 | 0 | LEU B | 252 | | .011 | | 73.071 | 1.00 20.14 |
| ATOM | 5025 | N | LEU B | 500 | | | | 73.911 | 1.00 20.33 |
| MOTA | 5026 | CA | LEU B | 253 | | .057 | | | 1.00 15.18 |
| ATOM | 5027 | CB | LEU B | 253 | | .304 | | | 1.00 18.34 |
| MOTA | 5028 | CG | LEU B | | | .490 | | 73.688 | 1.00 14.11 |
| ATOM | 5029 | CD1 | LEU B | 253 | | .062 | | 74.829 | 1.00 10 50 |
| ATOM | 5030 | CD2 | LEU B | 253 | | . 552 | | 72.624 | 1.00 19.60 |
| ATOM | 5031 | C | LEU B | 253 | | .550 | | 74.536 | 1.00 20.54 |
| ATOM | 5032 | Š | LEU B | | | .200 | | 73.821 | 1.00 22.80 |
| | 5033 | N | GLN B | 254 | 53 | .495 | -3.858 | 75.865 | 1.00 20.37 |
| ATOM | 5034 | CA | GLN B | | | .000 | | 76.539 | 1.00 21.77 |
| ATOM | | CB | GLN B | | | .129 | | 77.755 | 1.00 17.85 |
| ATOM | 5035 | | GLN E | | | .724 | | 79.124 | 1.00 32.51 |
| ATOM | 5036 | CG | | | | .563 | | 79.609 | 1.00 28.19 |
| ATOM | 5037 | CD | GLN E | | | .507 | | 80.124 | 1.00 26.96 |
| ATCM | 5038 | OEI | GLN E | 474 | | .603 | | 79.432 | |
| ATOM | 5039 | NE2 | GLN E | 454 | 53 | | -0.012 | | |

| | | | | | 76 007 | 1.00 20.15 |
|------|------|---------------|----------|--------|--------|------------|
| MOTA | 5040 | C GLN B 254 | 54.211 | -1.793 | 76.887 | |
| MOTA | 5041 | O GLN B 254 | 55.186 | -2.254 | 77.497 | 1.00 20.11 |
| | 5042 | N LEU B 255 | 54.146 | -0.532 | 76.468 | 1.00 19.46 |
| ATOM | _ | | 55.268 | 0.386 | 76.614 | 1.00 15.99 |
| ATOM | 5043 | CA LEU B 255 | 55.692 | 0.831 | 75.211 | 1.00 18.15 |
| ATOM | 5044 | CB LEU B 255 | - | | 74.296 | 1.00 21.80 |
| ATOM | 5045 | CG LEU B 255 | 56.143 | -0.316 | | |
| MCTA | 5046 | CD1 LEU B 255 | 56.215 | 0.159 | 72.850 | 1.00 16.70 |
| | 5047 | CD2 LEU B 255 | 57.501 | -0.843 | 74.771 | 1.00 13.76 |
| ATOM | | | 55.083 | 1.614 | 77.492 | 1.00 21.41 |
| MOTA | 5048 | C LEU B 255 | 55.379 | 2.741 | 77.065 | 1.00 18.40 |
| MOTA | 5049 | O _LEU B 255 | | 1.408 | 78.718 | 1.00 16.80 |
| ATOM | 5050 | N GLY B 256 | 54.618 | | | 1.00 19.90 |
| ATOM | 5051 | CA GLY B 256 | 54.456 | 2.519 | 79.634 | |
| ATOM | 5052 | C GLY B 256 | · 55.816 | 3.181 | 79.818 | 1.00 17.68 |
| | 5053 | O GLY B 256 | 56.854 | 2.514 | 79.841 | 1.00 13.96 |
| ATOM | | | 55.824 | 4.497 | 79.936 | 1.00 19.55 |
| MOTA | 5054 | N THR B 257 | 57.081 | 5.205 | 80.098 | 1.00 19.47 |
| ATOM | 5055 | CA THR B 257 | | 6.547 | 79.340 | 1.00 21.49 |
| ATOM | 5056 | CB THR B 257 | 57.044 | | | 1.00 17.43 |
| MCTA | 5057 | OG1 THR B 257 | 55.989 | 7.365 | 79.858 | |
| ATOM | 5058 | CG2 THR B 257 | 56.780 | 6.311 | 77.850 | 1.00 22.49 |
| | 5059 | C THR B 257 | 57.440 | 5.466 | 81.564 | 1.00 20.75 |
| ATOM | | 553 | 58.480 | 5.054 | 81.843 | 1.00 25.01 |
| MOTA | 5060 | | 56.618 | 5.004 | 82.504 | 1.00 17.23 |
| ATOM | 5061 | | _ | 5.277 | 83.906 | 1.00 17.42 |
| ATOM | 5062 | CA ASP B 258 | 56.929 | | | 1.00 12.75 |
| MOTA | 5063 | CB ASP B 258 | 55.744 | 4.940 | 84.846 | 1.00 12.75 |
| ATOM | 5064 | CG ASP B 258 | 55.197 | 3.524 | 84.676 | |
| ATOM | 5065 | C ASP B 258 | 58.245 | 4.718 | 84.460 | 1.00 16.09 |
| | 5066 | O ASP B 258 | 58.667 | 5.116 | 85.542 | 1.00 22.07 |
| ATOM | - | OD1 ASP B 258 | 55.901 | 2.642 | 84.150 | 1.00 17.74 |
| ATOM | 5067 | ODI ASP B 258 | 54.041 | 3.281 | 85.109 | 1.00 18.68 |
| atom | 5068 | OD2 ASP B 258 | | 3.746 | 83.779 | 1.00 20.98 |
| ATOM | 5069 | N PRO B 259 | 58.879 | | | 1.00 17.75 |
| ATOM | 5070 | CD PRO B 259 | 58.474 | 2.901 | 82.641 | |
| ATOM | 5071 | CA PRO B 259 | 60.154 | 3.257 | 84.321 | 1.00 22.63 |
| | 5072 | CB PRO B 259 | 60.395 | 1.988 | 83.506 | 1.00 23.46 |
| ATOM | _ | | 59.800 | 2.343 | 82.199 | 1.00 27.08 |
| ATOM | 5073 | | | 4.284 | 84.172 | 1.00 23.86 |
| ATOM | 5074 | | 62.406 | 4.082 | 84.698 | 1.00 24.24 |
| ATOM | 5075 | O PRO B 259 | | | 83.465 | 1.00 20.49 |
| ATOM | 5076 | N LEU B 260 | 61.054 | 5.387 | | 1.00 15.17 |
| ATOM | 5077 | CA LEU B 260 | 62.080 | 6.417 | 83.262 | 1.00 13.17 |
| ATOM | 5078 | CB LEU B 260 | 61.626 | 7.408 | 82.185 | 1.00 17.03 |
| | 5079 | CG LEU B 260 | 61.431 | 6.881 | 80.760 | 1.00 16.02 |
| MOTA | | CD1 LEU B 260 | 60.703 | 7.915 | 79.901 | 1.00 17.03 |
| ATOM | 5080 | | 62.803 | 6.546 | 80.163 | 1.00 18.58 |
| ATOM | 5081 | | 62.449 | 7.194 | 84.541 | 1.00 22.45 |
| ATOM | 5082 | C LEU B 260 | | | 85.412 | 1.00 17.84 |
| ATOM | 5083 | O LEU B 260 | 61.611 | 7.440 | | 1.00 22.90 |
| ATOM | 5084 | N LEU B 261 | 63.713 | 7.588 | 84.635 | |
| | 3085 | CA LEU B 261 | 64.219 | 8.332 | 85.782 | 1.00 26.34 |
| ATOM | 5086 | CB LEU B 261 | 65.605 | 8.914 | 85.473 | 1.00 20.58 |
| ATOM | | | 66.180 | 9.850 | 86.553 | 1.00 28.44 |
| ATOM | 5087 | | 66.481 | 9.055 | 87.812 | 1.00 29.84 |
| ATOM | 5088 | CD1 LEU B 261 | | 10.522 | 86.057 | 1.00 32.10 |
| ATOM | 5089 | CD2 LEU B 261 | 67.462 | | | 1.00 27.61 |
| ATOM | 5090 | C LEU B 261 | 63.315 | 9.475 | 86.227 | |
| ATOM | 5091 | O LEU B 261 | 62.978 | 9.586 | 87.408 | 1.00 24.02 |
| | 5092 | N GLU B 262 | 62.934 | 10.315 | 85.269 | 1.00 23.33 |
| ATOM | | | 62.126 | 11.490 | 85.530 | 1.00 23.38 |
| ATOM | 5093 | | 62.115 | 12.415 | 84.302 | 1.00 23.17 |
| MOTA | 5094 | CB GLU B 262 | | 12.854 | 83.806 | 1.00 28.98 |
| ATOM | 5095 | CG GLU B 262 | 63.503 | | | 1.00 32.26 |
| ATOM | 5096 | CD GLU B 262 | 64.179 | 11.831 | 82.902 | |
| ATOM | 5097 | CE1 GLU B 262 | 63.702 | 10.673 | 82.838 | 1.00 29.28 |
| | 5098 | OE2 GLU B 262 | 65.201 | 12.186 | 82.264 | 1.00 25.42 |
| ATOM | | | 60.693 | 11.249 | 85.976 | 1.00 23.25 |
| ATOM | 5099 | | 60.013 | 12.192 | 86.368 | 1.00 27.63 |
| ATCM | 5100 | O GLU B 262 | | | | 1.00 22.25 |
| ATOM | 5101 | N ASP B 263 | 60.219 | 10.011 | | |
| ATOM | 5102 | CA ASP B 263 | 58.840 | 9.751 | 86.345 | |
| ATOM | 5103 | CB ASP B 263 | 58.214 | 8.659 | 85.465 | |
| | 5104 | | 56.710 | 8.543 | | |
| ATOM | | | 55.995 | 8.318 | | 1.00 21.82 |
| ATOM | 5105 | ODI MOE D 200 | 32.233 | -, | • | |

| | | | | | 56.239 | 8.666 | 86.811 | 1.00 18.31 |
|--------|-------|------|----------------------------|----------|--------|--------|--------|------------|
| MOTA | 5106 | OD2 | ASP B 263 | | | | | |
| | 5107 | С | ASP B 263 | • | 58.834 | 9.339 | 87.814 | |
| MOTA | - | | | | 59.437 | 8.335 | 88.179 | 1.00 22.11 |
| ATOM | 5108 | 0 | ASP B 263 | | | | | 1.00 25.81 |
| ATOM | 5109 | N | TYR B 264 | | 58.155 | 10.124 | 88.648 | |
| | | | | | 58.101 | 9.864 | 90.084 | 1.00 30.96 |
| MOTA | 5110 | CA | | | | | | 1.00 36.80 |
| | 5111 | CB | TYR B 264 | | 57.511 | 11.055 | 90.841 | |
| ATOM | | | | | 58.241 | 12.356 | 90.645 | 1.00 46.58 |
| MOTA | 5112 | CG | TYR B 264 | | | | | |
| | 5113 | CD1 | TYR B 264 | | 57.981 | 13.166 | 89.542 | |
| MOTA | | | | | 58.654 | 14.370 | 89.364 | 1.00 50.25 |
| ATOM | 5114. | CE1 | TYR B 264 | | | | | 1.00 50.94 |
| ATOM | 5115 | CD2 | TYR B 264 | | 59.197 | 12.779 | 91.565 | |
| | | | TYR B 264 | | 59.876 | 13.977 | 91.396 | 1.00 51.28 |
| MOTA | 5116 | CE2 | | | | | 90.297 | 1.00 52.21 |
| ATOM | 5117 | CZ | TYR B 264 | | 59.600 | 14.769 | | |
| | | | TYR B 264 | | 60.268 | 15.961 | 90.142 | 1.00 49.65 |
| ATOM | 5118 | ОН | | | | | 90.525 | 1.00 31.04 |
| MOTA | 5119 | С | TYR B 264 | | 57.340 | 8.628 | | |
| | | 0 | TYR B 264 | | 57.514 | 8.181 | 91.657 | 1.00 24.50 |
| MOTA | 5120 | | | | 56.491 | 8.074 | 89.666 | 1.00 26.68 |
| MOTA | 5121 | N | LEU B 265 | | | | | 1.00 24.17 |
| ATOM | 5122 | CA | LEU B 265 | | 55.744 | 6.900 | 90.086 | |
| | | | LEU B 265 | | 54.371 | 6.838 | 89.390 | 1.00 24.69 |
| MOTA | 5123 | CB | LEU B 20- | | | | 89.761 | 1.00 26.00 |
| ATOM | 5124 | CG | LEU B 265 | | 53.415 | 7.982 | | |
| | 5125 | CD1 | LEU B 265 | | 51.970 | 7.583 | 89.460 | 1.00 22.21 |
| ATOM . | - | | 110 D 200 | | 53.530 | 8.281 | 91.238 | 1.00 29.31 |
| ATOM | 5126 | CD2 | LEU B 265 | | | | | 1.00 25.83 |
| | 5127 | С | LEU B 265 | | 56.478 | 5.568 | 89.948 | |
| MOTA | | | LEU B 265 | | 55.848 | 4.512 | 89.908 | 1.00 21.74 |
| ATOM | 5128 | 0 | TEO B 703 | ' | | | | 1.00 23.30 |
| MOTA | 5129 | N | SER B 266 | | 57.808 | 5.618 | 89.867 | |
| | | - | SER B 266 | | 58.608 | 4.398 | 89.813 | 1.00 20.75 |
| ATOM | 5130 | CA | | | | | 88.378 | 1.00 19.67 |
| ATOM | 5131 | CB | SER B 266 | 1 | 58.820 | 3.900 | | 1.00 19.01 |
| | 5132 | . OG | SER B 266 | ; | 59.863 | 4.615 | 87.739 | 1.00 18.11 |
| ATOM | | | | | | 4.710 | 90.420 | 1.00 23.01 |
| ATOM | 5133 | С | SER B 266 | | 59.963 | | | 1.00 17.74 |
| | 5134 | 0 | SER B 266 | ; | 60.437 | 5.845 | 90.345 | |
| ATOM | | | | | 60.590 | 3.707 | 91.023 | 1.00 24.25 |
| MOTA | 5135 | N | | | | | 91.613 | 1.00 23.79 |
| MOTA | 5136 | CA | LYS B 26 | | 61.905 | 3.916 | | 1.00 25.75 |
| | | | LYS B 26 | , | 62.027 | 3.153 | 92.929 | 1.00 23.71 |
| MOTA | 5137 | CB | | | | 3.582 | 93.960 | 1.00 27.29 |
| ATOM | 5138 | CG | LYS B 26 | | 60.989 | | | 1.00 30.33 |
| | 5139 | CD | LYS B 26 | 7 | 61.059 | 5.088 | 94.207 | 1.00 30.33 |
| ATOM | | | 7.7.C D 36' | , | 60.067 | 5.535 | 95.273 | 1.00 30.90 |
| ATOM | 5140 | CE | LYS B 26 | _ | | | 95.509 | 1.00 33.37 |
| ATOM | 5141 | NZ | LYS B 26 | 7 | 60.155 | 7.004 | | |
| | | | LYS B 26 | | 62.990 | 3.483 | 90.634 | 1.00 26.41 |
| MOTA | 5142 | С | | | 64.153 | 3.317 | 91.016 | 1.00 25.33 |
| ATOM | 5143 | 0 | LYS B 26 | | | | | 1.00 22.18 |
| | 5144 | N | PHE B 26 | 3 | 62.595 | 3.288 | 89.375 | |
| MOTA | | | | | 63.529 | 2.919 | 88.318 | 1.00 22.78 |
| ATOM | 5145 | CA | | | | 2.171 | 87.179 | 1.00 20.55 |
| MOTA | 5146 | CB | PHE B 26 | 3 | 62.814 | | | |
| | | CG | PHE B 26 | 3 | 62.389 | 0.761 | 87.526 | 1.00 19.23 |
| MOTA | 5147 | | | | 61.722 | -0.025 | 86.585 | 1.00 20.72 |
| ATOM | 5148 | CD | PHE B 26 | | | | | 1.00 18.17 |
| MOTA | 5149 | CD2 | PHE B 26 | 3 | 62.673 | 0.207 | 88.773 | |
| | | 000 | PHE B 26 | | 61.344 | -1.336 | 86.875 | 1.00 18.83 |
| MOTA | 5150 | CE | L PRE 5 20 | _ | | | 89.073 | 1.00 20.05 |
| ATOM | 5151 | CE2 | PHE B 26 | 3 | 62.300 | -1.105 | | 1.0' 19.70 |
| | 5152 | CZ | PHE B 26 | 8 | 61.634 | -1.879 | 88.122 | |
| ATOM · | | | 200 2 26 | | 64.114 | 4.222 | 87.785 | 1.00 23.66 |
| ATOM | 5153 | С | PHE B 26 | . | | | | 1.00 19.40 |
| ATOM | 5154 | 0 | PHE B 26 | В | 63.412 | 5.232 | 87.692 | 1.00 13.40 |
| | | | ASN B 26 | a | 65.396 | 4.203 | 87.437 | 1.00 21.96 |
| ATOM | 5155 | N | ASN B ZO | _ | | 5.396 | 86.926 | 1.00 25.04 |
| MOTA | 5156 | СA | ASN B 26 | 9 | 66.060 | | | 1 00 25 65 |
| | | CB | ASN B 26 | 9 | 67.243 | 5.783 | 87.824 | 1.00 25.68 |
| ATOM | 5157 | | ASN 5 30 | _ | 66.845 | 5.946 | 89.273 | 1.00 27.04 |
| ATOM | 5158 | CG | ASN B 26 | 7 | | | | 1.00 28.81 |
| ATOM | 5159 | OD. | 1 ASN B 26 | 9 | 65.832 | 6.557 | 89.579 | 1.00 20.01 |
| | | | 2 ASN B 26 | ۵ | 67.659 | 5.419 | 90.176 | 1.00 31.12 |
| ATOM | 5160 | | ADN B 40 | _ | | | 85.523 | 1.00 25.87 |
| ATOM | 5161 | С | ASN B 26 | 9 | 66.579 | 5.151 | | |
| | | | ASN B 26 | | 67.769 | 5.336 | 85.268 | 1.00 24.58 |
| ATOM | 5162 | 0 | 7211 5 20 | _ | | 4.757 | 84.611 | 1.00 21.37 |
| ATOM | 5163 | N | LEU B 27 | U | 65.695 | | 02.041 | 1.00 16.35 |
| | | ÇA | | 0 | 66.116 | 4.462 | 83.241 | |
| MOTA | 5164 | | | _ | 65.176 | 3.426 | 82.610 | 1.00 24.12 |
| ATOM | 5165 | CB | LEU B 27 | U | | | 83.412 | 1.00 27.89 |
| | 5166 | CG | LEU B 27 | 0 | 64.909 | | | |
| ATOM | | ~~ | 1 LEU B 27 | 0 | 64.181 | 1.136 | 82.515 | 1.00 23.03 |
| ATOM | 5167 | Ω٦ | <u>، نہ</u> ⊂ ∪حب <u>ہ</u> | • | | | | |
| ATOM | 5168 | CD | 2 LEU B 27 | U | 66.221 | | | |
| | 5169 | | LEU B 27 | 0 | 66.184 | 5.682 | 82.337 | |
| ATOM | | | | | 65.654 | | 82.663 | 1.00 16.3 |
| ATOM | 5170 | | LEU B 27 | | | | | |
| ATOM | 5171 | | SER B 27 | 1 | 66.839 | 5.497 | - | 1.00 |
| AIUH | | | _ | | | | _ | |
| | | | | | | | | |

| | | | | | • | | | | |
|-----------|------|-----|-------|-----|--------|--------|---------|------|-------|
| \ | 5172 | CA | SER B | 271 | 66.989 | 6.546 | 80.200 | 1.00 | 21.20 |
| MOTA | | | SER B | | 68.437 | 6.621 | 79.714 | | 21.80 |
| MOTA | 5173 | CB | | | 68.772 | 5.485 | 78.921 | | 21.47 |
| MOTA | 5174 | OG | SER B | | | 6.228 | 79.000 | | 22.83 |
| ATOM | 5175 | С | | 271 | 66.106 | | | | 16.12 |
| ATOM | 5176 | 0 | SER B | | 65.631 | 5.102 | 78.854 | | |
| ATOM | 5177 | Ŋ | ASN B | 272 | 65.916 | 7.238 | 78.154 | | 20.84 |
| ATOM | 5178 | CA | ASN B | 272 | 65.152 | 7.156 | 76.906 | _ | 27.82 |
| ATOM | 5179 | CB | ASN B | 272 | 65.263 | 8.478 | 76.123 | | 30.30 |
| ATOM | 5180 | CG | | 272 | 64.198 | 9.456 | 76.475 | | 37.83 |
| | 5181 | OD1 | • | | 64.167 | 10.575 | 75.946 | | 37.72 |
| MOTA | 5182 | | | 272 | 63.299 | 9.052 | 77.360 | 1.00 | 41.69 |
| ATOM | | | ASN B | | 65.701 | 6.088 | 75.974 | 1.00 | 26.88 |
| ATOM | 5183 | C | ASN B | | 64.967 | 5.280 | 75.412 | 1.00 | 23.12 |
| MOTA | 5184 | 0 | | | 67.012 | 6.160 | 75.774 | | 20.40 |
| MOTA | 5185 | N | | 273 | 67.745 | 5.260 | 74.899 | _ | 27.34 |
| MOTA | 5186 | CA | VAL B | | | 5.705 | 74.805 | | 30.40 |
| ATOM | 5187 | CB | VAL B | | 69.225 | | 74.029 | | 34.98 |
| ATOM | 5188 | | | 273 | 70.036 | 4.691 | | | 33.57 |
| MOTA | 5189 | | VAL B | | 69.299 | 7.057 | 74.115 | | 24.23 |
| ATOM | 5190 | С | | 273 | 67.664 | 3.812 | 75.343 | | |
| ATOM | 5191 | 0 | | 273 | 67.590 | 2.913 | 74.513 | | 24.19 |
| MOTA | 5192 | N | ALA B | 274 | 67.690 | 3.580 | 76.648 | | 20.96 |
| ATOM | 5193 | CA | ALA B | 274 | 67.589 | 2.220 | 77.151 | | 18.12 |
| ATOM | 5194 | CB | ALA B | 274 | 67.858 | 2.195 | 78.646 | | 19.09 |
| ATOM | 5195 | c | | 274 | 66.172 | 1.729 | 76.863 | | 18.23 |
| ATOM | 5196 | ō | | 274 | 65.962 | 0.567 | 76.525 | 1.00 | 20.77 |
| | 5197 | N | PHE B | | 65.207 | 2.631 | 77.003 | 1.00 | 18.50 |
| ATOM | 5198 | CA | | 275 | 63.802 | 2.310 | 76.761 | 1.00 | 21.25 |
| MOTA | | CB | PHE B | | 62.941 | 3.546 | 77.037 | 1.00 | 22,24 |
| ATOM | 5199 | | | 275 | 61.466 | 3.303 | 76.921 | 1.00 | 24.72 |
| ATOM | 5200 | CG | | 275 | 60.815 | 2.483 | 77.826 | | 23.64 |
| MOTA | 5201 | CD1 | | | 60.732 | 3.893 | 75.907 | | 27.31 |
| MOTA | 5202 | CD2 | PHE B | | 59.450 | 2.254 | 77.722 | | 27.82 |
| MOTA | 5203 | CE1 | PHE B | | | 3.670 | 75.795 | | 27.62 |
| MOTA | 5204 | CE2 | PHE B | | 59.365 | | 76.701 | | 25.78 |
| MOTA | 5205 | CZ | PHE B | | 58.727 | 2.851 | 75.305 | | 24.47 |
| ATOM | 5206 | С | | 275 | 63.642 | 1.860 | | | |
| ATOM | 5207 | 0 | PHE B | 275 | 63.045 | 0.821 | 75.030 | 1.00 | |
| ATOM | 5208 | N | | 276 | 64.183 | 2.648 | 74.378 | | 23.85 |
| MOTA | 5209 | CA | LEU B | 276 | 64.128 | 2.330 | 72.946 | | 21.28 |
| ATOM | 5210 | CB | LEU B | 276 | 64.814 | 3.421 | 72.134 | 1.00 | |
| MOTA | 5211 | CG | LEU B | 276 | 65.114 | 3.132 | 70.662 | | 24.94 |
| MOTA | 5212 | CD1 | LEU B | 276 | 63.818 | 2.852 | 69.936 | | 24.81 |
| MOTA | 5213 | CD2 | LEU B | 276 | 65.840 | 4.312 | 70.018 | | 21.01 |
| MOTA | 5214 | C | LEU B | 276 | 64.841 | 1.021 | 72.653 | | 22.33 |
| MOTA | 5215 | ŏ | | 276 | 64.348 | 0.191 | 71.886 | | 20.73 |
| | 5216 | N | LYS B | | 66.011 | 0.857 | 73.261 | | 20.72 |
| ATOM | 5217 | CA | LYS 3 | | 66.823 | -0.335 | 73.076 | 1.00 | 24.36 |
| ATOM | | CB | LYS B | | 68.086 | -0.239 | 73.938 | 1.00 | 27.37 |
| ATOM | 5218 | CG | LYS 3 | | 69.303 | -0.973 | 73.381 | 1.00 | 35.58 |
| ATOM | 5219 | | LYS B | | 69.061 | -2.456 | 73.188 | | 43.87 |
| ATOM | 5220 | CD | | | 70.283 | -3.137 | 72.580 | | 44.87 |
| ATOM | 5221 | CE | LYS B | | | -2.586 | 71.230. | 1.00 | 49.66 |
| MOTA | 5222 | NZ | LYS B | | 70.616 | -1.554 | 73.482 | 1 00 | 24.22 |
| MOTA | 5223 | С | LYS B | | 66.000 | | 72.777 | | 19.90 |
| ATOM | 5224 | 0 | LYS B | | 65.987 | -2.568 | 74.624 | 1.00 | 22.32 |
| MOTA | 5225 | N | ALA B | | 65.319 | -1.454 | | 1.00 | 21.71 |
| ATOM | 5226 | CA | ALA B | 278 | 64.476 | -2.544 | 75.114 | 1.00 | 17 24 |
| MOTA | 5227 | CB | ALA B | 278 | 63.752 | -2.117 | 76.381 | 1.00 | 17.34 |
| MOTA | 5228 | С | ALA B | 278 | 63.459 | -2.896 | 74.031 | 1.00 | 22.68 |
| ATOM | 5229 | Ö | ALA B | | 63.231 | -4.068 | 73.723 | 1.00 | 19.27 |
| ATOM | 5230 | N | PHE B | | 62.849 | -1.862 | 73.464 | 1.00 | 24.79 |
| | 5231 | CA | PHE B | | 61.860 | -2.014 | 72.398 | 1.00 | 22.74 |
| ATOM | | CB | PHE B | | 61.395 | -0.629 | 71.955 | 1.00 | 22.46 |
| ATOM | 5232 | | PHE B | | 60.467 | -0.640 | 70.778 | 1.00 | 22.62 |
| ATOM | 5233 | CG | | | 59.196 | -1.182 | 70.882 | 1.00 | 21.74 |
| MOTA | 5234 | | PHE B | | 60.862 | -0.078 | 69.567 | | 26.07 |
| MOTA | 5235 | | PHE B | | | -1.162 | 69.799 | | 27.02 |
| ATOM | 5236 | | PHE B | | 58.325 | -0.051 | 68.476 | | 25.57 |
| ATOM | 5237 | CE2 | PHE B | 279 | 60.001 | -0.031 | | | |

| | | | PHE B | 270 | 58.727 | -0.594 | 68.592 | 1.00 25 | 13 |
|-------|--------|------|---------|-------|----------|---------|--------|---------|-------------|
| ATOM | 5238 | CZ | | | | | | 1.00 23 | |
| ATOM | 5239 | Ç | PHE B | 279 | 62.472 | -2.768 | 71.212 | | |
| | | | PHE B | 279 | 61.866 | -3.697 | 70.678 | 1.00 26 | .54 |
| MOTA | 5240 | 0 | | | | | 70.804 | 1.00 21 | 93 |
| ATOM | 5241 | N | ASN B | 280 | 63.677 | -2.376 | | | |
| | | CA | ASN B | 280 | 64.318 | -3.046 | 69.680 | 1.00 23 | .70 |
| MOTA | 5242 | | | | | | 69.164 | | 2.63 |
| MOTA | 5243 | CB | ASN B | 280 | 65.520 | -2.248 | | | |
| | | CG | ASN B | 280 | 65.107 | -0.937 | 68.505 | 1.00 30 |).83 |
| MOTA. | 5244 | | | | | | 67.796 | 1.00 25 | 81 |
| MOTA | 5245 | OD1 | ASN B | 280 | 64.094 | -0.878 | | | |
| | 5246 | MT)2 | ASN B. | 280 | 65.900 | 0.112 | 68.714 | 1.00 26 | 5.54 |
| MOTA | | | YOM D. | 200 | | -4.466 | 70.009 | 1.00 26 | 10 |
| MOTA | 5247 | С | ASN B | 280 | 64.746 | | | | |
| | 5248 | 0 | ASN B | 280 - | 64.775 | -5.321 | 69.124 | 1.00 26 | .16 |
| MOTA | | | | | | -4.724 | 71.272 | 1.00 26 | 5.10 |
| ATOM | 5249 | N | ILE B | 781 | 65.080 | | | | |
| | 5250 | CA | ILE B | 281 | 65.485 | -6.067 | 71.667 | 1.00 25 | |
| ATOM | | | T. D. D | -01 | 66.006 | -5.098 | 73.124 | 1.00 28 | 3.50 |
| ATOM | 5251 | CB | ILE B | 201 | | | | | 3.53 |
| ATOM | 5252 | CG2 | ILE B | 281 | 66.046 | -7.527 | 73.648 | | |
| | | | ILE B | | 67.392 | -5.454 | 73.173 | 1.00 32 | 2.07 |
| MOTA | 5253 | CG1 | | | | | 74.541 | 1.00 28 | 3.24 |
| MOTA | 5254 | CD1 | ILE B | 281 | 68.038 | -5.442 | | | |
| | 5255 | С | ILE B | 281 | 64.320 | -7.030 | 71.507 | 1.00 25 |).// |
| ATOM | | | | | 64.484 | -8.131 | 70.982 | 1.00 23 | 3.39 |
| MOTA | 5256 | 0 | | 281 | | | | 1.00 2 | |
| MOTA | 5257 | N | VAL B | 282 | 63.139 | -6.618 | 71.950 | 1.00 2. | 1.30 |
| | | | VAL B | 282 | 61.961 | -7.465 | 71.813 | 1.00 22 | 2.90 |
| ATOM | 5258 | CA | | | | | 72.387 | 1.00 24 | |
| MOTA | 5259 | CB | VAL B | 282 | 60.703 | -6.775 | | | |
| | 5260 | CG1 | | 282 | 59.464 | -7.611 | 72.093 | 1.00 2 | 2.28 |
| ATOM | | | | | .60.865 | -6.587 | 73.906 | 1.00 20 | 5.89 |
| ATOM | 5261 | CG2 | | 282 | | | | | |
| MOTA | 5262 | С | VAL B | 282 | 61.718 | -7.795 | 70.339 | 1.00 2 | |
| | | | | 282 | 61.462 | -8.949 | 69.978 | 1.00 2 | 2.65 |
| MOTA | 5263 | 0 | | | | | | | 3.19 |
| ATOM | 5264 | N | ARG B | 283 | 61.799 | -6.779 | 69.488 | | |
| | | CA | | 283 | 61.576 | -6.971 | 68.060 | 1.00 2 | 7.95 |
| MOTA | 5265 | | | | 61.510 | -5.612 | 67.359 | 1.00 2 | 5.48 |
| MOTA | 5266 | CB | ARG B | 283 | | | | 1.00 2 | |
| | 5267 | CG | ARG B | 283 | 60.337 | -4.760 | 67.838 | 1.00 2 | |
| MOTA | | | | | 60 442 | 3.333 | 67.339 | 1.00 3 | 1.52 |
| ATOM | 5268 | CD | ARG B | 203 | | | | 1.00 2 | |
| ATOM | 5269 | NE | ARG B | 283 | 60.210 | -3.208 | 65.908 | | |
| | | CZ | ARG B | 283 | 60.915 | -2.414 | 65.116 | 1.00 2 | 6.45 |
| MOTA | 5270 | | ANG D | 203 | | -1.676 | 65.622 | 1.00 2 | 6 04 |
| ATOM | 5271 . | NH1 | ARG B | 283 | 61.902 | | | - 00 - | 0.01 |
| ATOM | 5272 | NH2 | ARG B | 283 | 60.634 | -2.356 | 63.825 | 1.00 2 | |
| | | | | | 62.634 | -7.855 | 67.402 | 1.00 3 | 2.04 |
| ATOM | 5273 | С | ARG B | 483 | | | | 1.00 2 | |
| MOTA | 5274 | 0 | ARG B | 283 | 62.341 | -8.552 | 66.431 | 1.00 2 | 9.70 |
| | | | | 284 | 63.859 | -7.821 | 67.923 | 1.00 3 | 1.50 |
| MOTA | 5275 | N | | | | -8.646 | 67.381 | 1.00 3 | 2.42 |
| ATOM | 5276 | CA | GLU B | 284 | 64.934 | | | | |
| ATOM | 5277 | CB | GLU B | 284 | 66.289 | -8.260 | 67.992 | 1.00 3 | 8.31 |
| | | | | | 66.798 | -6.864 | 67.640 | 1.00 4 | 8.93 |
| ATOM | 5278 | CG | | 284 | | | | 1.00 5 | |
| MOTA | 5279 | CD | GLU B | 284 | 68.102 | -6.518 | 68.362 | 1.00 5 | 0.20 |
| | 5280 | OE1 | | 284 | 69.084 | -7.281 | 68.222 | 1.00 5 | 7.37 |
| MOTA | | | | | | -5.485 | 69.069 | 1.00 5 | 5.42 |
| ATOM | 5281 | OE2 | GLU B | | 68.150 | | | | |
| ATOM | 5282 | С | GLU B | 284 | 64.638 | -10.105 | 67.714 | 1.00 3 | 1.93 |
| | | | GLU B | | 64 899 | -11.001 | 66.913 | 1.00 2 | 8.26 |
| ATOM | 5283 | 0 | | | | | | 1.00 2 | 8 09 |
| ATOM | 5284 | N | VAL B | 285 | | -10.340 | 68.901 | 1.00 2 | 0.00 |
| | 5285 | CA | VAL B | 285 | 63.765 | -11.697 | 69.325 | 1.00 3 | 0.67 |
| ATOM | | | | | | -11.802 | 70.863 | 1.00 2 | 8.33 |
| ATOM | 5286 | CB | VAL B | | | | | 1.00 2 | |
| ATOM | 5287 | CG1 | VAL B | 285 | 63.257 | -13.206 | 71.262 | | |
| | | 553 | VAL B | 2.85 | 65 037 | -11.470 | 71.478 | 1.00 2 | 6.93 |
| MOTA | 5288 | CGZ | VAL B | 255. | | | | 1.00 3 | 1 19 |
| ATOM | 5289 | С | VAL B | 285 | | -12.265 | 68.758 | | |
| | | ō | VAL B | | 62.422 | -13.423 | 68.349 | 1.00 3 | |
| ATOM | 5290 | | VAL D | 205 | | -11.460 | 68.729 | 1.00 2 | 8.21 |
| ATOM | 5291 | N | PHE B | 286 | | | | 1 00 3 | E 71 |
| MOTA | 5292 | CA | PHE B | 286 | 60.105 | -11.948 | 68.249 | 1.00 2 | |
| | | | 2112 2 | 236 | | -11.853 | 69.374 | 1.00 2 | 4.57 |
| ATOM | 5293 | CB | | | | | | 1.00 2 | 6 87 |
| ATOM | 5294 | CG | PHE B | 286 | 59.311 | -12.804 | 70.514 | 1.00 2 | |
| | | 201 | PHE B | 286 | 59,651 | -12.331 | 71.779 | 1.00 2 | .D.16 |
| MOTA | 5295 | | | 200 | | -14.180 | 70.319 | 1.00 2 | 2.51 |
| ATCM | 5296 | CD2 | PHE B | 286 | | | | 1.00 | 2 22 |
| | 5297 | CE1 | PHE B | | 59.880 | -13.213 | 72.833 | 1.00 2 | . 2 . 3 2 |
| ATOM | | | | 225 | | -15.063 | 71.362 | 1.00 2 | 1.99 |
| ATOM | 5298 | CE2 | PHE 3 | _ 30 | | | | 1.00 2 | 6.75 |
| ATOM | 5299 | CZ | PHE B | 286 | 59.772 | -14.578 | 72.626 | 1.00 4 | , , , , , |
| | | | PHE B | 286 | 1 59.518 | -11.318 | 66.993 | 1.00 2 | 15.90 |
| ATOM | 5300 | C | rne p | 200 | | | 66.620 | 1.00 2 | 22.84 |
| ATOM | 5301 | 0 | PHE B | 200 | | -11.630 | | 1.00 2 | 2 27 |
| | 5302 | N | GLY B | 287 | 60.272 | -10.451 | 66.329 | 1.00 | , , , , , , |
| ATOM | | | GLY B | 287 | 59.756 | | 65.130 | 1.00 2 | 8 د . د ي |
| ATOM | 5303 | CA | GTI D | 20, | 22.720 | | • | | |

| | | | | | | | | 1 20 20 17 |
|--------|------|-----|----------|-------|--------|--------|--------|------------|
| ATCM | 5304 | С | GLY B 2 | 287 | 58.765 | -8.719 | 65.498 | 1.00 29.17 |
| ATCM | 5305 | 0 | GLY B 2 | 287 | 58.786 | -8.216 | 56.517 | 1.00 22.88 |
| | 5306 | N | GLU B 2 | | 57.896 | -8.361 | 64.558 | 1.00 26.77 |
| ATCM | | | | | 56.893 | -7.324 | 64.754 | 1.00 25.38 |
| ATOM | 5307 | CA | GLU B 2 | | | -6.791 | 63.405 | 1.00 29.51 |
| MOTA | 5308 | CB | GLU B 2 | | 56.405 | | | |
| ATCM | 5309 | CG | GLU B 2 | 288 | 57.430 | -6.003 | 62.605 | 1.00 36.06 |
| | 5310 | CD | GLU B.2 | | 57.906 | -4.769 | 63.347 | 1.00 41.10 |
| ATCM | | | GLU B 2 | | 57.058 | -4.055 | 63.919 | 1.00 41.19 |
| ATCM | 5311 | OEI | GLU D 2 | .00 | 59.125 | -4.503 | 63.348 | 1.00 44.69 |
| ATCM | 5312 | | GLU B 2 | 288 | | | 65.527 | 1.00 27.87 |
| MOTA | 5313 | C | -GLU B 2 | | 55.682 | -7.819 | | |
| ATOM | 5314 | 0 . | GLU B 2 | 288 | 55.209 | -8.931 | 65.308 | 1.00 26.80 |
| ATOM | 5315 | N | GLY B 2 | | 55.176 | -6.973 | 66.419 | 1.00 24.53 |
| | 5316 | CA | GLY B 2 | | 54.006 | -7.326 | 67.204 | 1.00 29.17 |
| ATCM | | | | 289 | 53.015 | -6.171 | 67.244 | 1.00 30.46 |
| ATCM | 5317 | С | | | | -5.326 | 66.358 | 1.00 26.17 |
| ATOM | 5318 | 0 | GLY B 2 | | 53.005 | | - | 1.00 23.95 |
| ATOM | 5319 | N | | 290 | 52.171 | -6.142 | 68.268 | |
| ATCM | 5320 | CA | VAL B 2 | 290 | 51.194 | -5.079 | 68.440 | 1.00 22.25 |
| ATOM | 5321 | CB | VAL B | 290 | 49.794 | -5.655 | 68.783 | 1.00 18.71 |
| | 5322 | | | 290 | 48.810 | -4.525 | 69.047 | 1.00 22.67 |
| ATOM | | | | 290 | 49.289 | -6.504 | 67.629 | 1.00 19.26 |
| ATOM | 5323 | | | | 51.722 | -4.232 | 69.593 | 1.00 21.55 |
| ATCM | 5324 | С | | 290 | | | 70.687 | 1.00 21.32 |
| ATOM | 5325 | 0 | | 290 | 51.960 | -4.741 | | |
| ATCM | 5326 | N | TYR B | 291 | 51.913 | -2.941 | 69.346 | 1.00 21.06 |
| ATOM | 5327 | CA | TYR B | 291 | 52.479 | -2.063 | 70.357 | 1.00 19.29 |
| ATOM | 5328 | CB | TYR B | 291 | 53.582 | -1.216 | 69.711 | 1.00 20.40 |
| | 5329 | CG | TYR B | | 54.553 | -2.072 | 68.918 | 1.00 23.09 |
| MOTA | | | TYR B | | 54.740 | -1.875 | 67.549 | 1.00 19.52 |
| ATOM | 5330 | CD1 | | | 55.580 | -2.712 | 66.809 | 1.00 20.67 |
| ATOM | 5331 | CE1 | TYR B | 291 | 55.234 | -3.122 | 69.527 | 1.00 22.88 |
| ATOM | 5332 | CD2 | TYR B | 291 | | | 68.800 | 1.00 26.04 |
| MOTA | 5333 | CE2 | TYR B | 291 . | 56.070 | -3.960 | | 1.00 23.44 |
| ATOM · | 5334 | CZ | TYR B | 291 | 56.235 | -3.752 | 67.442 | |
| ATOM | 5335 | OH | TYR B | 291 | 57.027 | -4.612 | 66.722 | 1.00 28.02 |
| | 5336 | С | TYR B | 291 | 51.465 | -1.180 | 71.068 | 1.00 26.89 |
| ATOM | 5337 | õ | TYR B | | 50.668 | -0.479 | 70.429 | 1.00 20.26 |
| ATOM | | | LEU B | 202 | 51.522 | -1.204 | 72.399 | 1.00 21.75 |
| ATCM | 5338 | N | LEU B | 202 | 50.604 | -0.426 | 73.227 | 1.00 22.11 |
| ATOM | 5339 | CA | | | 49.765 | -1.369 | 74.088 | 1.00 20.92 |
| ATOM | 5340 | CB | LEU B | | | -2.542 | 73.375 | 1.00 22.94 |
| ATOM | 5341 | CG | LEU B | | 49.091 | | | 1.00 21.03 |
| MCTA | 5342 | CD1 | LEU B | 292 | 48.328 | -3.362 | 74.411 | |
| ATOM | 5343 | CD2 | LEU B | 292 | 48.149 | -2.043 | 72.281 | 1.00 18.04 |
| ATOM | 5344 | С | LEU B | | 51.330 | 0.557 | 74.147 | 1.00 21.59 |
| | 5345 | õ | LEU B | | 52.514 | 0.404 | 74.426 | 1.00 19.96 |
| ATOM | | N | GLY B | | 50.606 | 1.571 | 74.613 | 1.00 23.31 |
| ATOM | 5346 | | | 293 | 51.195 | 2.537 | 75.521 | 1.00 20.76 |
| ATOM | 5347 | CA | | | 51.163 | 1.979 | 76.930 | 1.00 26.15 |
| ATOM | 5348 | С | GLY B | | | 0.765 | 77.133 | 1.00 20.96 |
| ATOM | 5349 | 0 | GLY B | | 51.263 | | | |
| ATOM | 5350 | N | GLY B | 294 | 51.017 | 2.859 | 77.914 | 1.00 24.63 |
| ATOM | 5351 | CA | GLY B | 294 | 50.980 | 2.407 | 79.293 | 1.00 20.00 |
| ATCM | 5352 | C | GLY B | | 51.176 | 3.538 | 80.285 | 1.00 22.59 |
| | | ō | GLY B | | 51.145 | 4.719 | 79.916 | 1.00 17.46 |
| ATOM | 5353 | | GLY B | 295 | 51.373 | 3.179 | 81.551 | 1.00 17.10 |
| ATOM | 5354 | N | GLIS | 205 | 51.577 | 4.180 | 82.582 | 1.00 16.52 |
| ATOM | 5355 | CA | GLY B | 295 | | 5.145 | 82.232 | 1.00 19.54 |
| ATOM | 5356 | C | GLY B | 295 | 52.695 | | | 1.00 16.31 |
| ATOM | 5357 | o | GLY B | | 53.738 | 4.737 | 81.732 | 1.00 21.93 |
| ATOM | 5358 | N | GLY B | 296 | 52.467 | 6.430 | 82.497 | |
| ATOM | 5359 | ÇA | GLY B | 296 | 53.448 | 7.465 | 82.207 | 1.00 20.05 |
| | 5360 | c | GLY B | 296 | 52.869 | 8.750 | 82.759 | 1.00 22.20 |
| ATOM | | | GLY B | 296 | 51.790 | 9.160 | 82.336 | 1.00 20.48 |
| ATOM | 5361 | 0 | TYR B | 297 | 53.573 | 9.402 | 83.682 | 1.00 20.93 |
| ATOM | 5362 | N | TYK B | 207 | 53.025 | 10.598 | 84.306 | 1.00 23.25 |
| ATOM | 5363 | CA | TYR B | 23/ | | | 85.774 | 1.00 19.93 |
| ATOM | 5364 | CB | TYR 3 | 297 | 52.731 | 10.284 | 85.900 | 1.00 24.76 |
| ATOM, | 5365 | CG | TYR B | 297 | 52.041 | 8.944 | | 1.00 21.97 |
| ATOM | 5366 | CDI | TYR B | 297 | 52.779 | 7.758 | 85.936 | 1.00 21.37 |
| ATOM | 5367 | CE: | TYR B | 297 | 52.148 | 6.514 | 85.912 | 1.00 19.79 |
| | 5368 | כח: | TYR B | 297 | 50.653 | 8.850 | 85.849 | 1.00 20.86 |
| ATOM | | CE: | | 297 | 50.012 | 7.612 | 85.822 | 1.00 19.57 |
| ATOM | 5369 | دت. | | | | | • | |

| | | | | _ | | | 451 | 1 00 00 05 |
|------|------|------|-----------|---|--------|-----------|--------|------------|
| ATOM | 5370 | CZ | TYR B 297 | | 50.758 | 6.457 | 85.851 | 1.00 23.85 |
| | 5371 | OH | TYR B 297 | | 50.106 | 5.254 | 85.806 | 1.00 17.83 |
| MOTA | | | TYR B 297 | | 53.839 | 11.877 | 84.181 | 1.00 25.22 |
| MOTA | 5372 | С | TIN D 207 | | 53.451 | 12.925 | 84.705 | 1.00 21.77 |
| MOTA | 5373 | 0 | TYR B 297 | | 54.974 | 11.794 | 83.497 | 1.00 23.21 |
| ATOM | 5374 | | HIS B 298 | | | 12.976 | 83.270 | 1.00 25.62 |
| ATOM | 5375 | CA | HIS B 298 | | 55.787 | | 83.534 | 1.00 22.88 |
| ATOM | 5376 | СВ | HIS B 298 | | 57.270 | 12.713 | | |
| ATOM | 5377 | CG | HIS B 298 | | 58.097 | 13.956 | 83.502 | 1.00 25.13 |
| | 5378 | CD2 | HIS B 298 | | 58.406 | 14.791 | 82.482 | 1.00 28.22 |
| MOTA | 5379 | ומוא | HIS B 298 | | 58.617 | 14.536 | 84.641 | 1.00 32.76 |
| MOTA | | CEI | HIS B 298 | | 59.209 | 15.674 | 84.323 | 1.00 26.52 |
| ATOM | 5380 | 727 | HIS B 298 | | 59.094 | 15.852 | 83.019 | 1.00 32.15 |
| ATOM | 5381 | | | | 55.589 | 13.307 | 81.795 | 1.00 25.66 |
| MOTA | 5382 | C | | | 56.087 | 12.589 | 80.923 | 1.00 25.84 |
| MOTA | 5383 | 0 | HIS B 298 | | 54.901 | 14.424 | 81.496 | 1.00 27.02 |
| ATOM | 5384 | N | PRO B 299 | | - | 15.424 | 82.447 | 1.00 29.91 |
| MOTA | 5385 | CD | PRO B 299 | | 54.388 | | 80.127 | 1.00 26.53 |
| ATOM | 5386 | CA | PRO B 299 | | 54.616 | 14.864 | 80.342 | 1.00 27.76 |
| MOTA | 5387 | CB | PRO B 299 | | 53.952 | 16.232 | | 1.00 27.97 |
| ATOM | 5388 | CG | PRO B 299 | | 54.583 | 16.696 | 81.656 | 1.00 27.08 |
| ATOM | 5389 | С | PRO B 299 | | 55.815 | 14.930 | 79.194 | 1.00 27.00 |
| ATOM | 5390 | 0 | PRO B 299 | | 55.738 | 14.472 | 78.057 | 1.00 28.58 |
| ATOM | 5391 | N | TYR B 300 | | 56.925 | 15.484 | 79.668 | 1.00 27.30 |
| | 5392 | CA | TYR B 300 | | 58.114 | 15.593 | 78.824 | 1.00 27.17 |
| ATOM | 5393 | CB | TYR B 300 | | 59.173 | 16.496 | 79.466 | 1.00 31.65 |
| MOTA | | CG | TYR B 300 | | 58,684 | 17.851 | 79.921 | 1.00 31.61 |
| MOTA | 5394 | | TYR B 300 | | 57.414 | 18.318 | 79.582 | 1.00 32.71 |
| MOTA | 5395 | CD1 | TYR B 300 | | 56.971 | 19.568 | 80.014 | 1.00 38.52 |
| MOTA | 5396 | CE1 | TYR B 300 | | 59.499 | 18.670 | 80.701 | 1.00 30.92 |
| MOTA | 5397 | CD2 | | | 59.072 | 19.917 | 81.138 | 1.00 32.13 |
| MOTA | 5398 | CE2 | TYR B 300 | | 57.808 | 20.361 | 80.795 | 1.00 39.17 |
| MOTA | | CZ | TYR B 300 | | | 21.585 | 81.252 | 1.00 43.90 |
| MOTA | 5400 | OH | TYR B 300 | | 57.374 | 14.218 | 78.572 | 1.00 25.20 |
| ATOM | 5401 | С | TYR B 300 | | 58.731 | | 77.445 | 1.00 25.15 |
| ATOM | 5402 | 0 | TYR B 300 | | 59.106 | 13.894 | 79.628 | 1.00 20.55 |
| ATOM | 5403 | N | ALA B 301 | | 58.845 | 13.419 | | 1.00 22.12 |
| ATOM | 5404 | CA | ALA B 301 | | 59.414 | 12.080 | 79.508 | 1.00 17.09 |
| MOTA | 5405 | CB | ALA B 301 | | 59.417 | 11.388 | 80.874 | 1.00 17.05 |
| ATOM | 5406 | С | ALA B 301 | | 58.608 | 11.260 | 78.505 | 1.00 13.20 |
| ATOM | 5407 | 0 | ALA B 301 | | 59.161 | 10.629 | 77.613 | |
| MOTA | 5409 | N | LEU B 302 | | 57.295 | 11.290 | 78.667 | 1.00 18.02 |
| MOTA | 5409 | CA | LEU B 302 | | 56.381 | 10.553 | 77.815 | 1.00 19.88 |
| MOTA | 5410 | CB | LEU B 302 | | 54.957 | 10.702 | 78.362 | 1.00 21.72 |
| | 5411 | CG | LEU B 302 | | 53.767 | 10.118 | 77.606 | 1.00 31.08 |
| MOTA | 5412 | CD1 | LEU B 302 | | 52.576 | 9.980 | 78.549 | 1.00 31.35 |
| MOTA | 5413 | CDI | LEU B 302 | | 53.434 | 11.011 | 76.415 | 1.00 27.11 |
| ATOM | | | LEU B 302 | | 56.445 | 10.988 | 76.351 | 1.00 21.13 |
| ATOM | 5414 | 2 | LEU B 302 | | 56.473 | 10.149 | 75.449 | 1.00 21.76 |
| ATOM | 5415 | 0 | ALA B 303 | | 56.472 | 12.293 | 76.115 | 1.00 17.69 |
| MOTA | 5416 | N | YEW B 202 | | 56.516 | 12.811 | 74.755 | 1.00 17.79 |
| MOTA | 5417 | CA | ALA B 303 | | 56.357 | 14.326 | 74.780 | 1.00 24.50 |
| ATOM | 5418 | CB | ALA B 303 | | 57.803 | 12.425 | 74.040 | 1.00 20.84 |
| ATOM | 5419 | С | ALA B 303 | - | 57.781 | 11.968 | 72.891 | 1.00 19.33 |
| MOTA | 5420 | 0 | ALA B 303 | | _ | 12.594 | 74.723 | 1.00 21.08 |
| MOTA | 5421 | N | ARG B 304 | | 58.930 | | 74.120 | 1.00 25.56 |
| MOTA | 5422 | CA | ARG B 304 | | 60.215 | 12.269 | | 1.00 18.37 |
| ATOM | 5423 | CB | ARG B 304 | | 61.375 | 12.825 | 74.962 | 1.00 23.12 |
| MOTA | 5424 | CG | ARG B 304 | | 61.427 | 14.356 | 75.072 | 1.00 29.00 |
| | 5425 | CD | ARG B 304 | | 62.797 | 14.758 | 75.624 | |
| ATOM | 5426 | NE | ARG B 304 | | 63.073 | 13.938 | 76.789 | 1.00 33.28 |
| ATOM | 5427 | C2 | ARG B 304 | | 64.271 | 13.689 | 77.283 | 1.00 30.24 |
| ATOM | | | | | 65.363 | 14.194 | 76.723 | |
| MOTA | 5428 | | | | 64.365 | 12.896 | 78.333 | 1.00 36.15 |
| ATOM | 5429 | | ARG B 304 | | 60.406 | | | 1.00 20.46 |
| ATOM | 5430 | | | | 60.850 | | | 1.00 18.70 |
| ATCM | 5431 | | ARG B 304 | | 60.070 | | | 1.00 22.48 |
| ATOM | 5432 | | ALA B 305 | | 60.226 | | | 1.00 19.70 |
| ATOM | | | ALA B 305 | | 59.847 | | | 1.00 24.24 |
| ATCM | 5434 | | ALA B 305 | | 59.407 | | | |
| ATOM | 5435 | C | ALA B 305 |) | 33.407 | , . 5 5 0 | - | |

| | | _ | | · E | 59.938 | 7.184 | 72.888 | 1.00 19.12 |
|--------|------|-----|-----------------|-------|--------|--------|--------|------------|
| ATOM | 5436 | 0 | ALA B 30 | | _ | | | 1.00 18.65 |
| MOTA | 5437 | N | TRP B 30 |)6 | 58.113 | 8.230 | 73.659 | |
| | | | TRP B 30 | 16 | 57.298 | 7.668 | 72.600 | 1.00 19.57 |
| ATOM | 5438 | CA | | | 55.800 | 7.856 | 72.893 | 1.00 18.26 |
| ATOM | 5439 | CB | TRP B 30 | | | | 73.953 | 1.00 20.71 |
| ATOM | 5440 | CG | TRP B 30 |)6 | 55.301 | 6.911 | | |
| | 5441 | CD2 | TRP B 30 |)6 | 54.087 | 7.025 | 74.708 | 1.00 23.94 |
| MOTA | | | | | 53.988 | 5.870 | 75.513 | 1.00 24.73 |
| MOTA | 5442 | CE2 | | | | 7.991 | 74.780 | 1.00 26.01 |
| ATOM | 5443 | CE3 | TRP B 30 |)6 | 53.073 | | | |
| ATOM | 5444 | CD1 | TRP B 30 |)6 | 55.872 | 5.721 | 74.326 | 1.00 20.04 |
| | | | TEP B 30 | | 55.092 | 5.093 | 75.260 | 1.00 19.17 |
| ATOM | 5445 | NE1 | | | 52.912 | 5.655 | 76.385 | 1.00 28.04 |
| ATOM | 5446 | CZ2 | TRP B 30 | | | | 75.646 | 1.00 28.68 |
| ATOM | 5447 | CZ3 | TRP B 30 | 06 | 52.001 | 7.779 | | |
| | 5448 | CH2 | TRP B 30 | 06 | 51.930 | 6.619 | 76.437 | 1.00 31.22 |
| MOTA | | | TRP B 30 | | 57.665 | 8.223 | 71.226 | 1.00 23.48 |
| MOTA | 5449 | C | | | 57.416 | 7.574 | 70.212 | 1.00 22.38 |
| ATOM | 5450 | 0 | | | | | 71.176 | 1.00 22.36 |
| MOTA | 5451 | N | THR B 30 | o7 · | 58.262 | 9.412 | | |
| ATOM | 5452 | CA | THR B 30 | 07 | 58.672 | 9.953 | 69.880 | 1.00 25.94 |
| | | ¢в | THR B 30 | 0.7 | 59.143 | 11.417 | 69.986 | 1.00 25.88 |
| ATOM | 5453 | | | | 58.015 | 12.261 | 70.258 | 1.00 21.07 |
| ATOM | 5454 | OG1 | | | | 11.864 | 68.686 | 1.00 22.52 |
| ATOM | 5455 | CG2 | | | 59.827 | | | |
| ATOM | 5456 | С | THR B 30 | 07 | 59.815 | 9.078 | 69.350 | |
| | 5457 | Ō | THR B 30 | 07 | 59.922 | 8.834 | 68.144 | 1.00 25.82 |
| MOTA | | | LEU B 30 | | 60.564 | 8.596 | 70.258 | 1.00 27.54 |
| ATOM | 5458 | Ŋ | 150 B 30 | 00 | 61.773 | 7.734 | 69.857 | 1.00 26.76 |
| MOTA | 5459 | CA | LEU B 30 | | | | | 1.00 24.24 |
| ATOM | 5460 | CB | LEU B 30 | 08 | 62.691 | 7.424 | 71.054 | |
| | 5461 | CG | LEU B 3 | 0.8 | 63.420 | 8.614 | 71.718 | 1.00 31.16 |
| MOTA | | | | | 64.282 | 8.147 | 72.877 | 1.00 24.71 |
| ATOM | 5462 | CD1 | | | | 9.325 | 70.700 | 1.00 24.59 |
| MOTA | 5463 | CD2 | | 80 | 64.289 | | | 1.00 27.20 |
| ATOM | 5464 | С | LEU B 30 | 08 | 61.184 | 6.443 | 69.287 | |
| | 5465 | 0 | | 08 | 61.609 | 5.961 | 68.234 | 1.00 23.52 |
| MOTA | | | | 09 | 60.190 | 5.898 | 69.980 | 1.00 25.10 |
| MOTA | 5466 | N | | | 59.537 | 4.679 | 69.530 | 1.00 25.14 |
| ATOM | 5467 | CA | | 09 | | | | 1.00 27.05 |
| ATOM | 5468 | CB | ILE B 3 | 09 | 58.387 | 4.266 | 70.485 | |
| | 5469 | CG2 | _ | 09 | 57.646 | 3.058 | 69.926 | 1.00 23.57 |
| ATOM | | CG1 | | 09 | 58.952 | 3.947 | 71.868 | 1.00 22.98 |
| MOTA | 5470 | | _ | | 59.927 | 2.793 | 71.868 | 1.00 24.25 |
| MOTA | 5471 | CD1 | | 09 | | 4.885 | 68.133 | 1.00 25.41 |
| ATOM | 5472 | С | | 09 | 58.958 | | | |
| ATOM | 5473 | 0 | ILE B 3 | 09 | 59.177 | 4.064 | 67.243 | |
| | 5474 | N | TRP B 3 | | 58.232 | 5.984 | 67.943 | 1.00 27.45 |
| MOTA | | | | 10 | 57.618 | 6.266 | 66.648 | 1.00 29.27 |
| ATOM | 5475 | CA | | | 56.721 | 7.505 | 66.715 | 1.00 27.00 |
| ATOM | 5476 | C3 | TRP B 3 | | | | 65.378 | 1.00 28.26 |
| MOTA | 5477 | CG | TRP B 3 | 10 | 56.112 | 7.847 | | |
| | 5478 | CD2 | TRP B 3 | 10 | 55.172 | 7.061 | 64.633 | 1.00 27.50 |
| MOTA | | CE | | 10 | 54.947 | 7.729 | 63.408 | 1.00 30.47 |
| ATOM | 5479 | | _ | | 54.500 | 5.856 | 64.877 | 1.00 29.85 |
| ATOM | 5480 | CE3 | _ | | | P.929 | 64.597 | 1.00 29.76 |
| MOTA | 5481 | CD: | TRP B 3 | | 56.406 | | | 1.00 26.71 |
| ATOM | 5482 | NE: | TRP B 3 | 10 | 55.713 | .865 | 63.415 | 1.00 20.71 |
| | 5483 | cz: | | 10 | 54.076 | .234 | 62.429 | 1.00 28.23 |
| MOTA | | | _ | | 53.636 | 5.362 | 63.901 | 1.00 30.24 |
| ATCM | 5484 | CZ | | | | 6.053 | 62.692 | 1.00 27.63 |
| ATOM | 5485 | CH | TRP B 3 | 10 | 53.433 | | | 1.00 30.16 |
| ATOM | 5486 | С | TRP B 3 | 10 | 58.629 | 6.424 | 65.520 | |
| | 5487 | ō | TRP B 3 | | 58.378 | 5.964 | 64.410 | 1.00 30.04 |
| ATOM | | | CYS B 3 | | 59.762 | 7.069 | 65.793 | 1.00 24.26 |
| ATCM | 5488 | N | _YS B 3 | 1 4 4 | | 7.233 | 64.764 | 1.00 27.97 |
| MOTA | 5489 | CA | CYS B 3 | | 60.782 | | | 1.00 28.21 |
| MOTA | 5490 | CB | CYS B 3 | 11 | 61.893 | 8.157 | 65.252 | |
| | 5491 | SG | CYS B 3 | 11 | 61.422 | 9.905 | 65.381 | 1.00 33.38 |
| ATOM | | | CYS B 3 | | 61.380 | 5.886 | 64.351 | 1.00 30.02 |
| MOTA | 5492 | Ċ | | | 61.670 | 5.660 | 63.172 | 1.00 25.45 |
| ATOM | 5493 | 0 | CYS B 3 | 7.7 | | | | 1.00 31.59 |
| ATOM | 5494 | N | GLU B 3 | 312 | 61.570 | 5.001 | 65.327 | |
| | 5495 | CA | GLU B 3 | | 62.111 | 3.669 | 65.067 | 1.00 33.48 |
| ATOM | | | GLU B 3 | | 62.142 | 2.843 | 66.352 | 1.00 34.78 |
| ATOM | 5496 | CB | 200 D 3 | 112 | | 2.307 | 66.758 | |
| ATOM | 5497 | CG | GLU B 3 | 14 | 63.487 | | | |
| ATOM | 5498 | CD | GLU B 3 | 312 | 64.171 | 1.513 | 65.675 | |
| ATOM | 5499 | | | 312 | 63.539 | 0.614 | 65.081 | |
| | | | GLU B 3 | 312 | 65.358 | 1.782 | 65.437 | 1.00 39.26 |
| , ATOM | 5500 | | د <u>م</u> ان ن | 112 | 61.197 | 2.959 | | |
| 2 TOM | 5501 | С | GLU B 3 | 14 | ロエ・エフィ | 2.933 | | |

| | | | | | - | | | |
|--------------|---------------|----------|--------------------------|---|------------------|------------------|------------------|--------------------------|
| ATOM | 5502 | 0 . | GLU B 312 | | 61.640 | | | 1.00 31.38 |
| ATOM | 5503 | N | LEU B 313 | | 59.919 | | | 1.00 26.70 1.00 26.73 |
| ATOM | 5504 | CA | LEU B 313 | | 58.930 | | 63.598 64.297 | 1.00 25.83 |
| MOTA | 5505 | | LEU B 313 | | 57.571 | 2.173 1.224 | 65.477 | 1.00 35.18 |
| MOTA | 5506 | | LEU B 313 | | 57.429 56.063 | 1.434 | 66.130 | 1.00 32.49 |
| MOTA | 5507 | CD1 | LEU B 313 | | | -0.215 | 64.989 | 1.00 29.71 |
| MOTA | 550.8 | CD2 | LEU B 313 LEU B 313 | | 58.768 | 2.866 | 62.248 | 1.00 29.03 |
| MOTA | 5509 5510 | С 0 | LEU B 313 | | 58.716 | 2.187 | 61.228 | 1.00 25.39 |
| ATOM ATOM | 5510 | N | SER B 314 | | 58.677 | 4.194 | 62.263 | 1.00 30.13 |
| ATOM | 5512 | CA | SER B 314 | - | 58.498 | 5.006 | 61.060 | 1.00 34.06 |
| ATOM | 5513 | CB | SER B 314 | | 58.206 | 6.456 | 61.445 62.234 | 1.00 31.15 1.00 48.58 |
| ATOM | 5514 | OG | SER B 314 | | 57.041 | 6.537 5.003 | 60.151 | 1.00 31.84 |
| MOTA | 5515 | C | SER B 314 | | 59.707 59.632 | 5.469 | 59.026 | 1.00 34.15 |
| ATOM | 5516 | 0 | SER B 314 GLY B 315 | | 60.831 | 4.515 | 60.655 | 1.00 31.81 |
| ATOM | 5517 5518 | N CA | GLY B 315 | | 62.036 | 4.485 | 59.848 | 1.00 37.27 |
| ATOM ATOM | 5519 | C | GLY B 315 | | 62.659 | 5.851 | 59.616 | 1.00 39.93 |
| ATOM | 5520 | ŏ | GLY B 315 | | 63.363 | 6.054 | 58.624 | 1.00 39.79 1.00 38.22 |
| ATOM | 5521 | N | ARG B 316 | | 62.422 | 6.798 | 60.518 60.336 | 1.00 38.22 1.00 38.66 |
| ATOM | 5522 | CA | ARG B 316 | | 63.004 61.908 | 8.121 9.184 | 60.275 | 1.00 40.20 |
| MOTA | 5523 | CB | ARG B 316 | | 61.908 | 9.345 | 61.520 | 1.00 39.00 |
| ATOM | 5524 | CG | ARG B 316 ARG B 316 | | 60.032 | 10.398 | 61.284 | 1.00 42.13 |
| ATOM | 5525 5526 | CD NE | ARG B 316 | | 59.002 | 9.954 | 60.352 | 1.00 45.09 |
| MOTA MOTA | 5527 | CZ | ARG B 315 | | 58.075 | 10.754 | 59.838 | 1.00 40.84 |
| ATOM | 5528 | NH1 | ARG B 316 | | 58.064 | 12.033 | 60.170 | 1.00 48.44 1.00 35.96 |
| ATOM | 5529 | NH2 | ARG B 316 | | 57.150 | 10.278 8.467 | 59.014 61.408 | 1.00 39.03 |
| MOTA | 5530 | C | ARG B 316 | | 64.031 63.952 | 7.988 | 62.539 | 1.00 34.34 |
| MOTA | 5531 | 0 | ARG B 316 GLU B 317 | | 65.003 | 9.296 | 61.035 | 1.00 39.58 |
| MOTA | 5532 | N CA | GLU B 317 | | 66.074 | 9.697 | 61.943 | 1.00 43.35 |
| MOTA MOTA | 5533 5534 | CB | GLU B 317 | | 67.142 | 10.509 | 61.203 | 1.00 49.34 |
| ATOM | 5535 | CG | GLU B 317 | | 67.609 | 9.910 | 59.884 | 1.00 57.04 1.00 62.79 |
| MOTA | 5536 | CD | GLU B 317 | | 66.546 | 10.009 | 58.798 58.467 | 1.00 63.46 |
| MOTA | 5537 | 0E1 | GLU B 317 | | 66.146 66.108 | 11.149 8.954 | 58.280 | 1.00 64.46 |
| ATOM | 5538 | OE2 | GLU B 317 GLU B 317 | | 65.555 | 10.528 | 63.100 | 1.00 41.58 |
| ATOM | 5539 | С 0 | GLU B 317 | | 64.658 | 11.356 | 62.939 | 1.00 39.74 |
| MOTA | 5540 5541 | И | VAL B 318 | | 66.118 | 10.301 | 64.278 | 1.00 35.38 |
| MOTA MOTA | 5542 | CA | VAL B 318 | | 65.706 | 11.049 | 65.448 | 1.00 38.76 1.00 42.28 |
| ATOM | 5543 | CB | VAL B 318 | | 66.000 | 10.265 | 66.750 67.962 | 1.00 38.26 |
| MOTA | 5544 | CG1 | VAL B 318 | | 65.560 65.287 | 11.080 8.916 | 66.722 | 1.00 39.99 |
| MOTA | 5545 | CG2 | VAL B 318 | | 66.459 | 12.370 | 65.478 | 1.00 41.82 |
| ATOM | 5546 | | VAL B 318 VAL B 318 | | 67.689 | 12.395 | 65.570 | 1.00 37.20 |
| MOT. | 5547 5548 | о 0 | PRO B 319 | | 65.735 | 13.491 | 65.356 | 1.00 43.18 |
| ATOM ATOM | 5549 | CD | PRO B 319 | | 64.290 | 13.672 | 65.155 | 1.00 41.90 1.00 44.31 |
| ATOM | 5550 | CA | PRO B 319 | | 66.402 | 14.792 | 65.388 65.181 | 1.00 44.58 |
| ATOM | 5551 | CB | PRO B 319 | | 65.241 | 15.763 15.011 | 65.795 | 1.00 43.34 |
| MOTA | 5552 | | PRO B 319 | | 64.079 67.086 | 14.965 | 66.741 | 1.00.44.62 |
| ATOM | 5553 | C | PRO B 319 PRO B 319 | | 66.541 | 14.565 | 67.771 | 1.00 43.75 |
| ATOM | 5554 | O N | GLU B 320 | | 68.277 | 15.552 | 66.735 | 1.00 44.16 |
| ATOM | .5555 5556 | | GLU B 320 | | 69.029 | 15.762 | 67.967 | 1.00 45.92 |
| MOTA MOTA | 5557 | | GLU B 320 | | 70.381 | 16.406 | 67.663 | |
| ATOM | 5558 | | GLU B 320 | | 71.165 | 16.768 | 68.919 68.620 | |
| ATOM | 5559 | CD | GLU B 320 | | 72.455 | 17.505 17.874 | | 1.00 56.37 |
| ATOM | 5560 | | 1 GLU B 320 | | 73.161 72.762 | 17.714 | | 1.00 60.07 |
| MOTA | 5561 | | 2 GLU B 320 GLU B 320 | | 68.311 | 16.625 | 68.995 | 1.00 44.42 |
| ATOM | 5562 | | GLU B 320 | | 68.244 | 16.279 | 70.168 | |
| ATOM | 5563 5564 | | LYS B 321 | | 67.778 | 17.753 | | |
| ATCM ATOM | 5565 | | LYS B 321 | | 67.102 | 18.672 | | |
| ATOM | 5566 | | LYS B 321 | | 67.853 | 20.000 | | |
| MOTA | 5567 | | | | 67.890 | 20.802 | . 00.19 | , 1.00 01.44 |
| | | | | | | | | |

| | | | | | | 20 111 | 67.057 | 1.00 57.24 |
|------|------|-----|---------|---------|----------|--------|---------|------------|
| ATOM | 5568 | CD | LYS B | 321 | 68.700 | 20.144 | - | |
| ATOM | 5569 | CE | LYS B | 321 | 67.936 | 19.062 | 66.280 | 1.00 55.24 |
| | | NZ | | 321 | 66.738 | 19.588 | 65.558 | 1.00 55.31 |
| MOTA | 5570 | | | | 65.662 | 18.971 | 69.098 | 1.00 43.44 |
| MOTA | 5571 | С | LYS B | | | | 67.978 | 1.00 43.03 |
| MOTA | 5572 | 0 | LYS B | 321 | 65.211 | 18.736 | | |
| MOTA | 5573 | N | LEU B | 322 | 64.947 | 19.512 | 70.076 | 1.00 39.45 |
| | | | LEU B | | 63.563 | 19.885 | 69.875 | 1.00 40.31 |
| ATOM | 5574 | CA | | | 62.846 | 20.034 | 71.215 | 1.00 40.88 |
| ATOM | 5575 | CB | | 322 | | | | 1.00 40.09 |
| ATOM | 5576 | CG | LEU B | 322 | 62.943 | 18.901 | 72.234 | |
| ATOM | 5577 | CDL | LEU B | 322 | 62.001 | 19.175 | 73.388 | 1.00 38.17 |
| | | | | 322 | 62.588 | 17.596 | 71.580 | 1.00 41.56 |
| ATOM | 5578 | | | | 63.615 | 21.244 | 69.197 | 1.00 41.23 |
| AŢOM | 5579 | С | | 322 | | | 69.531 | 1.00 39.22 |
| MOTA | 5580 | 0 | LEU B | 322 . | 64.466 | 22.070 | | |
| ATOM | 5581 | Ń | ASN B | 323 | 62.735 | 21.473 | 68.233 | 1.00 40.04 |
| | 5582 | CA | ASN B | 323 | 62.703 | 22.771 | 67.582 | 1.00 43.32 |
| ATOM | | | | 323 | 61.985 | 22.707 | 66.234 | 1.00 41.53 |
| MOTA | 5583 | CB | ASN B | | | 22.085 | 66.335 | 1.00 41.89 |
| ATOM | 5584 | CG | ASN B | 323 | 60.617 | | | 1.00 39.79 |
| ATOM | 5585 | OD1 | ASN B | 323 | 59.889 | 22.308 | 67.304 | |
| | 5586 | | ASN 3 | 323 | 60.243 | 21.317 | 65.317 | 1.00 40.43 |
| ATOM | | | ASN B | 323 | 61.949 | 23.690 | 68.532 | 1.00 44.76 |
| ATOM | 5587 | C | | | 61.402 | 23.237 | 69.539 | 1.00 45.80 |
| MOTA | 5588 | 0 | ASN B | 323 | | | 68.210 | 1.00 46.85 |
| ATOM | 5589 | N | ASN B | 324 | 61.902 | 24.973 | | |
| ATOM | 5590 | CA | ASN B | 324 | 61.234 | 25.930 | 69.076 | 1.00 47.60 |
| | 5591 | CB | ASN B | 324 | 61.460 | 27.348 | 68.549 | 1.00 50.87 |
| ATOM | | | | | 61.089 | 28.407 | 69.562 | 1.00 55.06 |
| ATOM | 5592 | CG | ASN B | 324 | | 28.565 | 69.919 | 1.00 60.68 |
| ATOM | 5593 | | ASN B | 324 | 59.925 | | | |
| ATOM | 5594 | ND2 | ASN B | 324 | 62.091 | 29.131 | 70.048 | 1.00 59.17 |
| | 5595 | С | ASN B | 324 | 59.740 | 25.664 | 69.249 | 1.00 43.97 |
| ATOM | | | ASN B | 324 | 59.190 | 25.898 | 70.322 | 1.00 41.33 |
| MOTA | 5596 | 0 | ASN 5 | 324 | 59.087 | 25.168 | 68.201 | 1.00 43.49 |
| ATOM | 5597 | N | LYS B | 325 | | | | 1.00 45.95 |
| ATOM | 5598 | CA | LYS B | 325 | 57.655 | 24.892 | 68.264 | |
| ATOM | 5599 | CB | LYS B | 325 | 57.112 | 24.415 | 66.909 | 1.00 48.97 |
| | | CG | LYS B | | 57.212 | 25.400 | 65.731 | 1.00 53.41 |
| ATOM | 5600 | | 113 D | 325 | 58.582 | 25.386 | 65.024 | 1.00 58.77 |
| MOTA | 5601 | CD | LYS B | 325 | | 26.013 | 65.846 | 1.00 58.10 |
| ATOM | 5602 | CE | LYS B | | 59.700 | | | 1.00 53.38 |
| MOTA | 5603 | NZ | LYS B | 325 | 61.024 | 25.906 | 65.178 | |
| ATOM | 5604 | С | LYS B | 325 | 57.368 | 23.822 | 69.309 | 1.00 45.79 |
| | | | LYS B | | 56.375 | 23.891 | 70.034 | 1.00 43.91 |
| ATOM | 5605 | 0 | | | 58.245 | 22.829 | 69.381 | 1.00 44.28 |
| ATOM | 5606 | N | ALA B | | | | 70.336 | 1.00 44.25 |
| ATOM | 5607 | CA | ALA B | | 58.078 | 21.746 | | 1.00 41.44 |
| ATOM | 5608 | CB | ALA B | 326 | 59.013 | 20.589 | 69.986 | |
| | 5609 | c | ALA B | | 58.342 | 22.233 | 71.757 | 1.00 40.92 |
| ATOM | | | | | 57.639 | 21.843 | 72.688 | 1.00 39.02 |
| ATOM | 5610 | 0 | ALA B | | 59.352 | 23.085 | 71.922 | 1.00 38.14 |
| ATOM | 5611 | N | LYS B | | | | 73.246 | 1.00 40.11 |
| ATOM | 5612 | CA | LYS B | 327 | 59.689 | 23.603 | | |
| ATOM | 5613 | CB | LYS E | 327 | 60.892 | 24.552 | 73.178 | 1.00 42.36 |
| | 5614 | CG | LYS E | | 62.174 | 23.922 | 72.: 59 | 1.00 45.78 |
| ATOM | | | LYS E | | 63.325 | 24.926 | 72.f 75 | 1.00 48.46 |
| ATOM | 5615 | CD | | | 64.594 | 24.367 | 72.031 | 1.00 49.62 |
| ATOM | 5616 | CE | LYS E | | | | | 1.00 48.53 |
| ATOM | 5617 | NZ | LYS E | 327 | 65.108 | 23.139 | 72.700 | |
| ATOM | 5618 | С | LYS E | | 58.500 | 24.338 | 73.841 | 1.00 39.17 |
| | 5619 | | LYS E | | 58.132 | 24.112 | 74.994 | 1.00 38.87 |
| ATOM | | 0 | D13 E | 720 | 57.898 | 25.215 | 73.048 | 1.00 41.06 |
| atom | 5620 | N | GLU E | | | 25.986 | 73.512 | 1.00 42.35 |
| ATOM | 5621 | CA | GLU E | | 56.750 | | | 1.00 44.02 |
| ATOM | 5622 | CB | GLU E | 3 3 2 8 | 56.357 | 27.028 | 72.463 | |
| | 5623 | ĊĠ | GLU E | | 57.434 | 28.084 | 72.258 | 1.00 44.80 |
| ATOM | | | | | 57.835 | 28.742 | 73.569 | 1.00 48.40 |
| ATOM | 5624 | כם | GLU E | | | 29.317 | 74.237 | 1.00 51.20 |
| ATOM | 5625 | | l GLU E | | 56.949 | | | 1.00 47.81 |
| ATOM | 5626 | OE: | GLU E | 3 328 | 59.029 | 28.680 | 73.935 | |
| | 5627 | c c | GLU E | | 55.569 | 25.087 | 73.839 | |
| ATOM | | | | | 54.794 | 25.377 | 74.750 | 1.00 41.20 |
| ATOM | 5628 | 0 | GLU : | | | 23.999 | 73.090 | |
| ATOM | 5629 | N | LEU : | | . 55.429 | | | |
| ATOM | 5630 | CA | LEU F | 3 329 | 54.349 | 23.056 | 73.334 | |
| | 5631 | CB | LEU I | 3 329 | 54.404 | 21.900 | 72.334 | |
| ATOM | | | LEU I | | 53.344 | | 72.544 | |
| ATOM | 5632 | CG | | | 51.958 | 21.430 | | |
| ATOM | 5633 | CD | 1 LEU ! | 5 329 | 31.336 | 22.300 | | |
| | | | | | | | | |

| | E C 2 A | CD2 | LEU B | 329 | 53.521 | 19.699 | 71.525 | 1.00 | |
|------|---------|------|-------|------------|--------|--------|--------|-------|---------|
| ATOM | 5634 | | DEU D | 220 | 54.504 | 22.507 | 74.747 | 1.00 | 34.07 |
| ATOM | 5635 | | LEU B | | 53.621 | 22.664 | 75.583 | 1.00 | |
| MOTA | 5636 | | LEU B | | | | 75.013 | 1.00 | |
| MOTA | 5637 | | LEU B | | 55.640 | 21.873 | | | |
| MOTA | 5638 | CA | LEU B | 330 | 55.889 | 21.311 | 76.330 | 1.00 | |
| | 5639 | | | 330 | 57.267 | 20.642 | 76.382 | 1.00 | |
| ATOM | | | LEU B | | 57.466 | 19.428 | 75.470 | 1.00 | 34.91 |
| MOTA | 5640 | CG | LEU 5 | 330 | 58.832 | 18.817 | 75.728 | 1.00 | 34.69 |
| ATOM | 5641 | CD1 | LEU B | 330 | | 18.396 | 75.742 | | 34.10 |
| ATOM | 5642 | CD2 | LEU B | 330 | 56.369 | | | 1.00 | |
| MOTA | 5643 | С | LEU B | 330 | 55.789 | 22.363 | 77.429 | | |
| MOTA | 5644 | 0 | LEU B | 330 | 55.210 | 22.110 | 78.482 | 1.00 | |
| | 5645 | | LYS B | | 56.353 | 23.540 | 77.186 | 1.00 | |
| MOTA | | | LYS B | | 56.313 | 24.604 | 78.181 | | 43.35 |
| MOTA | 5646 | CA | LYS B | 221 | 57.162 | 25.788 | 77.712 | 1.00 | 46.25 |
| MOTA | 5647 | CB | LIS B | 227 | 58.658 | 25.496 | 77.685 | 1.00 | 51.07 |
| MOTA | 5648 | | LYS B | | 59.482 | 26.610 | 77.021 | 1.00 | 49.96 |
| ATOM | 5649 | CD | LYS B | 331 | | | 77.733 | | 53.08 |
| MOTA | 5650 | CE | LYS B | 331 | 59.371 | 27.957 | | | 56.18 |
| ATOM | 5651 | NZ | LYS B | 331 | 58.013 | 28.569 | 77.662 | | |
| ATOM | 5652 | С. | LYS B | 331 | 54.892 | 25.069 | 78.494 | | |
| | 5653 | ō | LYS B | 331 | 54.588 | 25.416 | 79.631 | | |
| MOTA | - | | SER B | 332 | 54.018 | 25.056 | 77.492 | 1.00 | |
| ATOM | 5654 | N | | 332 | 52.639 | 25.502 | 77.679 | 1.00 | 46.58 |
| MOTA | 5655 | CA | SER B | | 51.975 | 25.751 | 76.329 | 1.00 | 48.75 |
| ATOM | 5656 | CB | SER B | | | 24.527 | 75.646 | 1.00 | 49.55 |
| ATOM | 5657 | OG | SER B | | 51.769 | | 78.451 | 1.00 | 49.56 |
| ATOM | 5658 | С | SER B | 332 | 51.780 | 24.507 | | | 46.67 |
| ATOM | 5659 | 0 | SER B | 332 | 50.618 | 24.791 | 78.749 | | |
| ATOM | 5660 | N | ILE B | | 52.341 | 23.345 | 78.770 | | 50.55 |
| | 5661 | CA | ILE B | 333 | 51.586 | 22.326 | 79.488 | | 51.93 |
| MOTA | | CB | ILE B | 333 | 52.259 | 20.945 | 79.376 | | 51.82 |
| ATOM | 5662 | | ILE B | 333 | 51.447 | 19.902 | 80.134 | 1.00 | 50.29 |
| MOTA | 5663 | CG2 | 175 5 | 222 | 52.359 | 20.539 | 77.905 | 1.00 | 52.18 |
| ATOM | 5664 | CG1 | ILE B | 333 | | 19.210 | 77.693 | 1.00 | 55.42 |
| MOTA | 5665 | CD1 | ILE B | 333 | 53.044 | | 80.964 | 1.00 | 51.45 |
| ATOM | 5666 | C | ILE B | 333 | 51.367 | 22.634 | | | 50.96 |
| ATOM | 5667 | 0 | ILE B | 333 - | 52.180 | 23.290 | 81.614 | | |
| ATOM | 5668 | N | ASP B | 334 | 50.245 | 22.141 | 81.472 | | 54.05 |
| ATOM | 5669 | CA | ASP B | | 49.850 | 22.306 | 82.865 | | 58.15 |
| | 5670 | CB | ASP B | | 48.320 | 22.216 | 82.959 | | 60.38 |
| MOTA | | | ASP B | 331 | 47.751 | 20.972 | 82.262 | | 63.85 |
| MOTA | 5671 | CG | | 224 | 48.017 | 19.833 | 82.710 | 1.00 | 59.16 |
| MOTA | 5672 | 9D1 | | | 47.033 | 21.138 | 81.252 | 1.00 | 59.71 |
| ATOM | 5673 | OD2 | | | | 21.207 | 83.701 | 1.00 | 55.47 |
| ATOM | 5674 | С | ASP E | | 50.506 | | 84.171 | 1 00 | 54.08 |
| ATOM | 5675 | 0 | ASP E | 3 3 3 4 | 49.833 | 20.291 | 83.906 | 1 00 | 54.60 |
| MOTA | 5676 | N | PHE E | 335 | 51.816 | 21.307 | | 1.00 | 56.60 |
| MOTA | 5677 | CA | PHE E | 3 3 3 5 | 52.524 | 20.266 | 84.641 | | |
| ATOM | 5678 | CB | PHE E | 3 3 3 5 | 53.718 | 19.784 | 83.811 | 1.00 | 53.01 |
| | 5679 | CG | | | 54.522 | 18.717 | 84.482 | | 49.30 |
| ATOM | | CG 1 | PHE E | | 53.898 | 17.589 | 85.008 | 1.00 | 45.61 |
| MOTA | 5680 | CDI | PRE | 335 | 55.901 | 18.843 | 84.605 | 1.00 | 46.83 |
| ATCM | 5681 | CDZ | PHE E | 3 333 | 54.637 | 16.600 | 85.651 | 1.00 | |
| MOTA | 5682 | CEl | PHE F | 3 3 3 5 | | 17.860 | 85.247 | | 46.02 |
| ATOM | 5683 | CE2 | PHE E | 3 335 | 56.651 | | 85.772 | 1 00 | 46.08 |
| MOTA | 5684 | CZ | PHE F | | 56.018 | 16.737 | | | 57.29 |
| ATOM | 5685 | С | PHE E | 3 3 3 5 | 52.971 | 20.559 | 86.072 | 1.00 | 57.23 |
| | 5686 | ō | PHE I | 3 3 3 5 | 52.197 | 20.378 | 87.012 | 1.00 | 63.54 |
| ATOM | 5687 | N | GLU I | 3 3 3 6 | 54.223 | 20.983 | 86.229 | | 55.21 |
| MOTA | | | CITI | 336 | 54.818 | 21.286 | 87.535 | 1.00 | 60.30 |
| MOTA | 5688 | CA | GLU A | 3 336 | 53.783 | 21.846 | 88.517 | 1.00 | 64.95 |
| MOTA | 5689 | CB | | B 336 | 54.375 | | 89.867 | | 71.50 |
| ATOM | 5690 | CG | GLU 1 | B 336 | | | 90.787 | | 75.37 |
| ATCM | 5691 | CD | GLU I | в 336 | 53.363 | | | | 75.32 |
| ATOM | 5692 | OE1 | GLU I | в 336 | 52.796 | | | | 76.84 |
| ATOM | 5693 | OE2 | | B 335 | 53.137 | | | | , ,0.04 |
| | 5694 | c | GLU | B 336 | 55.485 | 20.058 | | | 55.66 |
| ATOM | | | | B 336 | 54.823 | 19.093 | 88.529 | | 49.97 |
| ATOM | 5695 | | CTIT | B 337 | 56.807 | 20.125 | | | 54.26 |
| MOTA | 5696 | | G1-11 | 737 737 | 57.630 | | | | 54.35 |
| ATCM | 5697 | | | B 337 | 59.101 | | | 1.00 | 54.08 |
| ATOM | 5698 | CB | | B 337 | | | | | 54.15 |
| ATOM | 5699 | | GLU | B 337 | 60.074 | 18.315 | | . 2.0 | · - |

| 3.0034 | E700 | CD | GLU B | 337 | 59.856 | 17.496 | 87.259 | 1.00 48.94 |
|--------|------|-----|-------|-----|--------|--------|--------|-------------|
| MOTA | 5700 | | | | 59.958 | 18.049 | 86.142 | 1.00 41.06 |
| ATOM | 5701 | | - | 337 | | 16.292 | 87.391 | 1.00 50.23 |
| ATOM | 5702 | OE2 | | 337 | 59.581 | | | |
| MOTA | 5703 | С | GLU B | 337 | 57.278 | 18.740 | 90.227 | 1.00 55.08 |
| ATOM | 5704 | 0 | GLU B | 337 | 57.130 | 19.651 | 91.039 | 1.00 54.51 |
| | | | | 338 | 57.140 | 17.458 | 90.557 | 1.00 56.20 |
| ATOM | 5705 | N | | | | 17.048 | 91.918 | 1.00 57.73 |
| MOTA | 5706 | CA | | 338 | 56.798 | | | |
| MOTA | 5707 | CB | PHE B | 338 | 56.713 | 15.527 | 92.020 | 1.00 58.47 |
| ATOM | 5708 | CG | PHE B | 338 | 56.231 | 15.034 | 93.359 | 1.00 63.17 |
| | | CD1 | | 338 | 54.882 | 15.096 | 93.696 | 1.00, 64.86 |
| ATOM | 5709 | | | | 57.129 | 14.526 | 94.293 | |
| ATOM | 5710 | CD2 | | 338 | _ | | 94.943 | 1.00 65.25 |
| MOTA | 5711 | CE1 | | 338 | 54.434 | 14.656 | | |
| ATOM | 5712 | CE2 | PHE B | 338 | 56.693 | 14.087 | 95.539 | 1.00 63.64 |
| ATOM | 5713 | CZ | | 338 | 55.342 | 14.152 | 95.864 | 1.00 66.30 |
| | 5714 | Ċ | PHE B | | 57.836 | 17.539 | 92.918 | 1.00 61.85 |
| ATOM | | | | | 57.520 | 17.807 | 94.078 | 1.00 58.15 |
| ATOM | 5715 | 0 | PHE B | | | 17.636 | 92.466 | 1.00 64.63 |
| ATOM | 5716 | N | | 339 | 59.081 | | | 1.00 67.53 |
| ATOM | 5717 | CA | ASP B | | 60.167 | 18.099 | 93.316 | |
| ATOM | 5718 | CB | ASP B | 339 | 61.286 | 17.059 | 93.362 | 1.00 67.32 |
| ATOM | 5719 | CG | ASP B | 339 | 62.474 | 17.524 | 94.174 | 1.00 68.13 |
| | 5720 | | ASP B | | 62.280 | 17.909 | 95.346 | 1.00 68.68 |
| MOTA | | | ASE D | 220 | 63.603 | 17.502 | 93.646 | 1.00 69.03 |
| ATOM | 5721 | OD2 | ASP B | 333 | | 19.435 | 92.829 | 1.00 69.03 |
| MOTA | 5722 | С | ASP B | | 60.718 | | | |
| ATOM | 5723 | 0 | ASP B | 339 | 61.211 | 19.545 | 91.708 | 1.00 67.54 |
| ATOM | 5724 | N | ASP B | 340 | 60.626 | 20.442 | 93.693 | 1.00 72.19 |
| ATOM | 5725 | CA | | 340 | 61.088 | 21.797 | 93.402 | 1.00 75.20 |
| | 5726 | CB | | 340 | 61.113 | 22.623 | 94.689 | 1.00 77.04 |
| ATOM | | | | | 59.766 | 22.671 | 95.375 | 1.00 78.70 |
| ATOM | 5727 | CG | | 340 | | 23.181 | 94,763 | 1.00 79.66 |
| MOTA | 5728 | OD1 | | 340 | 58.803 | | | 1.00 80.53 |
| ATOM | 5729 | OD2 | | 340 | 59.668 | 22.194 | 96.525 | |
| MOTA | 5730 | Ċ | ASP B | 340 | 62.464 | 21.856 | 92.751 | 1.00 74.82 |
| ATOM | 5731 | 0 | ASP B | 340 | 62.615 | 22.400 | 91.659 | 1.00 78.48 |
| ATOM | 5732 | N | | 341 | 63.465 | 21.303 | 93.426 | 1.00 74.11 |
| | 5733 | CA | | 341 | 64.827 | 21.312 | 92.907 | 1.00 76.25 |
| MOTA | | | | 341 | 65.818 | 21.596 | 94.040 | 1.00 79.54 |
| MOTA | 5734 | CB | | | 67.277 | 21.653 | 93.596 | 1.00 82.33 |
| ATOM | 5735 | ÇG | | 341 | | | 92.577 | 1.00 83.24 |
| ATOM | 5736 | CD | | 341 | 67.539 | 22.750 | | 1.00 85.25 |
| ATOM | 5737 | OE1 | GLU B | 341 | 67.333 | 23.937 | 92.910 | |
| ATOM | 5738 | OE2 | GLU B | 341 | 67.950 | 22.427 | 91.443 | 1.00 83.72 |
| ATOM | 5739 | С | GLU B | 341 | 65.196 | 19.998 | 92.227 | 1.00 73.97 |
| ATOM | 5740 | ō | GLU B | | 65.627 | 19.051 | 92.883 | 1.00 77.10 |
| | 5741 | N | VAL B | | 65.033 | 19.946 | 90.910 | 1.00 71.92 |
| ATOM | | | | | 65.354 | 18.744 | 90.151 | 1.00 68.51 |
| MOTA | 5742 | CA | | 342 | | 18.027 | 89.663 | 1.00 68.83 |
| MOTA | 5743 | CB | | 342 | 64.081 | | | 1.00 67.57 |
| MOTA | 5744 | CG1 | VAL 3 | 342 | 63.268 | 17.552 | 90.837 | |
| ATOM | 5745 | CG2 | VAL B | 342 | 63.255 | 18.969 | 88.806 | 1.00 67.72 |
| ATOM | 5746 | С | VAL B | 342 | 66.201 | 19.059 | 88.927 | 1.00 65 35 |
| ATOM | 5747 | Ö | VAL B | | 67.177 | 18.366 | 88.640 | 1.00 68.31 |
| | | | ASP B | | 65.819 | 20.112 | 88.213 | 1.00 60.89 |
| MOTA | 5748 | N | | | 66.514 | 20.520 | 86.998 | 1.00 58.89 |
| ATOM | 5749 | CA | ASP B | | | | 87.223 | 1.00 63.48 |
| ATOM | 5750 | CB | ASP B | 343 | 68.024 | 20.636 | | |
| MOTA | 5751 | CG | ASP B | 343 | 68.763 | 21.070 | 85.966 | 1.00 66.69 |
| ATOM | 5752 | OD1 | ASP B | 343 | 70.012 | 21.070 | 85.970 | 1.00 67.64 |
| ATOM | 5753 | 002 | ASP B | 343 | 68.089 | 21.420 | 84.973 | 1.00 65.42 |
| | 5754 | c | ASP B | 343 | 66.264 | 19.499 | 85.900 | 1.00 53.17 |
| MOTA | | | ASP B | | 66.993 | 18.516 | 85.766 | 1.00 49.70 |
| MOTA | 5755 | 0 | | | | 19.735 | 85.124 | 1.00 50.24 |
| MOTA | 5756 | N | ARG B | 344 | 65.216 | 10.053 | 84.022 | 1.00 46.49 |
| MOTA | 5757 | CA | ARG B | 344 | 64.868 | 18.853 | | 1.00 40.43 |
| ATOM | 5758 | CB | ARG B | 344 | 63.467 | 18.269 | 84.228 | 1.00 42.41 |
| ATOM | 5759 | CG | ARG B | | 63.317 | 17.367 | 85.452 | 1.00 38.59 |
| | 5760 | CD | ARG B | | 64.344 | 16.246 | 85.432 | 1.00 37.12 |
| ATOM | | | ARG B | | 64.169 | 15.310 | 86.537 | 1.00 36.55 |
| ATOM | 5761 | NE | | | 65.078 | 14.413 | 86.905 | 1.00 37.20 |
| MOTA | 5762 | CZ | ARG B | | | 14.331 | 86.259 | 1.00 33.53 |
| ATOM | 5763 | | ARG B | | 66.234 | | 87.915 | 1.00 28.79 |
| ATOM | 5764 | NH2 | ARG B | | 64.830 | 13.595 | | 1.00 44.45 |
| ATOM | 5765 | C | ARG B | 344 | 64.910 | 19.660 | 82.732 | T.00 44.43 |
| | - | | | | | | - | |

| 3 mov | 5766 | 0 | ARG B 344 | 64.328 | 19.269 | 81.720 | 1.00 38.73 |
|-------|---------------|-----|--------------|----------|--------|---------|------------|
| ATOM | | | | 65.618 | 20.784 | 82.783 | 1.00 42.44 |
| ATOM | 5767 | N | - | 65.740 | 21.677 | 81.637 | 1.00 41.74 |
| ATOM | 5768 | CA | SER B 345 | | | | 1.00 43.47 |
| ATOM | 5769 | CB | SER B 345 | 66.661 | 22.849 | 81.993 | |
| | 5770 | OG | SER B 345 | 67.956 | 22.388 | 82.351 | 1.00 46.96 |
| MOTA | | | | 66.244 | 20.981 | 80.375 | 1.00 36.32 |
| ATOM | 5771 | С | | | | 79.273 | 1.00 35.70 |
| MOTA | 5772 | 0 | SER B 345 | 65.840 | 21.333 | | |
| ATOM | 5773 | N - | TYR B 346 | 67.117 | 19.992 | 80.534 | |
| | 5774 | CA | TYR B 346 | 67.661 | 19.264 | 79.391 | 1.00 34.77 |
| MOTA | _ | | TYR B 346 | 68.660 | 18.206 | 79.877 | 1.00 36.09 |
| MOTA | 5 7 75 | CB | | | 17.146 | 80.774 | 1.00 34.27 |
| ATOM | 5776 | ÇG | TYR B 346 | . 68.054 | | | 1.00 37.62 |
| ATOM | 5777 | CD1 | TYR B 346 | 67.433 | 16.013 | 80.240 | |
| | 5778 | CE1 | TYR B 346 | 66.843 | 15.048 | 81.077 | 1.00 36.73 |
| MOTA | | CD2 | TYR B 346 | 68.072 | 17.294 | 82.157 | 1.00 36.40 |
| ATOM | 5779 | | | 67.489 | 16.344 | 82.999 | 1.00 36.54 |
| ATOM | 5780 | CE2 | TYR B 346 | | | 82.45-7 | 1.00 36.54 |
| ATOM | 5781 | CZ | TYR B 346 | 66.878 | 15.228 | | |
| ATOM | 5782 | OH | TYR B 346 | 66.310 | 14.306 | 83.306 | |
| | 5783 | С | TYR B 346 | 66.563 | 18.599 | 78.570 | 1.00 36.26 |
| ATOM | | | TYR B 346 | 66.719 | 18.385 | 77.367 | 1.00 40.50 |
| MOTA | 5784 | 0 | | 65.445 | 18.282 | 79.214 | 1.00 32.72 |
| ATOM | 5785 | N | MET B 347 | | | 78.516 | 1.00 35.43 |
| ATOM | 5786 | CA | MET B 347 | 64.346 | 17.628 | | |
| ATOM | 5787 | CB | MET B 347 | 63.280 | 17.164 | 79.513 | 1.00 34.36 |
| | 5788 | CG | MET B 347 | 63.819 | 16.292 | 80.635 | 1.00 28.32 |
| MOTA | | | | 62.515 | 15.604 | 81.669 | 1.00 34.47 |
| MOTA | 5789 | SD | | 61.654 | 17.027 | 82.142 | 1.00 39.60 |
| ATOM | 5790 | CE | MET B 347 | | | 77.465 | 1.00 39.04 |
| MOTA | 5791 | С | MET B 347 | 63.701 | 18.525 | | |
| ATOM | 5792 | 0 | MET B 347 | 63.060 | 18.029 | 76.540 | 1.00 37.38 |
| | 5793 | N | LEU B 348 | 63.857 | 19.839 | 77.606 | 1.00 39.21 |
| MOTA | | | | 63.272 | 20.773 | 76.645 | 1.00 40.81 |
| MOTA | 5794 | CA | | | 22.058 | 77.339 | 1.00 36.87 |
| ATOM | 5795 | CB | LEU B 348 | 62.806 | | | 1.00 42.66 |
| MOTA | 5796 | ÇG | LEU B 348 | 61.690 | 21.975 | 78.384 | |
| ATOM | 5797 | | LEU B 348 | 61.507 | 23.337 | 79.032 | 1.00 43.41 |
| | | CD2 | | 60.391 | 21.511 | 77.741 | 1.00 40.47 |
| MOTA | 5798 | | | 64.289 | 21,133 | 75.573 | 1.00 41.13 |
| MOTA | 5799 | ,C | LEU B 348 | | 21.968 | 74.711 | 1.00 38.93 |
| MOTA | 5800 | 0 | LEU B 348 | 64.018 | | | 1.00 37.70 |
| ATOM | 5801 | N | GLU B 349 | 65.455 | 20.495 | 75.632 | |
| | 5802 | CA | GLU B 349 | 66.527 | 20.757 | 74.681 | 1.00 42.48 |
| MOTA | | | GLU B 349 | 67.856 | 20.953 | 75.422 | 1.00 45.02 |
| MOTA | 5803 | CB | | 67.834 | 22.035 | 76.493 | 1.00 53.82 |
| ATOM | 5804 | CG | GLU B 349 | | 23.402 | 75.938 | 1.00 57.46 |
| ATOM | 5805 | CD | GLU B 349 | 67.483 | | | 1.00 59.62 |
| ATOM | 5806 | OE1 | GLU B 349 | 68.211 | 23.885 | 75.044 | |
| | 5807 | OE2 | | 66.480 | 23.993 | 76.397 | 1.00 57.91 |
| MOTA | | | GLU B 349 | 66.709 | 19.638 | 73.664 | 1.00 43.57 |
| ATOM | 5808 | C | - | 66.577 | 19.849 | 72.459 | 1.00 41.26 |
| ATOM | 5809 | 0 | GLU B 349 | | 18.448 | 74.161 | 1.00 41.95 |
| ATOM | 5810 | N | THR B 350 | 67.027 | | | 1.00 40.02 |
| MOTA | 5811 | CA | THR B 350 | 67.264 | 17.299 | 73.298 | |
| | 5812 | CE | THR B 350 | 68.689 | 16.775 | 73.504 | 1.00 43.08 |
| MOTA | 5813 | | | 68.894 | 16.490 | 74.894 | 1.00 41.07 |
| ATOM | | OG1 | F 111V B 320 | 69.703 | 17.816 | 73.049 | 1.00 45.05 |
| ATOM | 5814 | CG2 | | | | 73.510 | 1.00 37.56 |
| ATOM | 5815 | C | THR B 350 | 66.278 | 16.154 | | 1.00 33.64 |
| MOTA | 5816 | 0 | THR B 350 | 65.754 | 15.966 | 74.611 | 1.00 33.04 |
| | 5817 | N | LEU B 351 | 66.043 | 15.391 | 72.445 | 1.00 32.86 |
| ATOM | | | LEU B 351 | 65.126 | 14.260 | 72.475 | 1.00 35.00 |
| MOTA | 5818 | CA | | 64.776 | 13.810 | 71.053 | 1.00 31.61 |
| MOTA | 5819 | CB | LEU B 351 | | 14.601 | 70.312 | 1.00 35.31 |
| MOTA | 5820 | CG | LEU B 351 | 63.709 | _ | | 1.00 37.88 |
| ATOM | 5821 | CD: | 1 LEU B 351 | 63.552 | 14.064 | 68.904 | 1.00 37.86 |
| | 5822 | CD | | 62.397 | 14.474 | 71.068 | 1.00 39.36 |
| ATOM | | | | 65.662 | 13.065 | 73.240 | 1.00 33.33 |
| MOTA | 5823 | С | LEU B 351 | | 12.469 | 74.046 | 1.00 31.48 |
| MOTA | 5824 | O | LEU B 351 | 64.956 | | | 1.00 29.58 |
| ATOM | 5825 | N | LYS B 352 | 66.915 | 12.720 | 72.981 | 1.00 22.30 |
| aton | 5826 | | LYS B 352 | 67.527 | 11.576 | 73.633 | 1.00 36.77 |
| | | | LYS B 352 | 68.457 | 10.864 | 72.647 | 1.00 34.32 |
| ATCM | 5827 | | 712 D 225 | 67.777 | 10.563 | 71.326 | 1.00 39.29 |
| ATOM | 5828 | | | | 9.949 | 70.294 | 1.00 42.25 |
| ATOM | 5829 | CD | | 68.703 | | | 1.00 46.22 |
| ATOM | 5830 | | | 69.110 | 8.541 | | |
| | 5831 | | | 69.831 | 7.905 | 69.516 | 1.00 44.15 |
| atom | 7071 | | | | | • | |

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| | | _ | 5 353 | | 68.295 | 11.983 | 74.878 | 1.00 36.30 |
|--------|------|------|-------------|---|--------|----------|--------|------------|
| ATOM | 5832 | С | LYS B 352 | | | | 74.865 | 1.00 36.65 |
| ATOM | 5833 | 0 | LYS B 352 | | 69.086 | 12.931 | | |
| | 5834 | N | ASP B 353 | | 68.049 | 11.275 | 75.967 | 1.00 30.01 |
| MOTA | | | ASP B 353 | | 68.757 | 11.569 | 77.188 | 1.00 33.99 |
| ATOM | 5835 | CA | | | | 11.308 | 78.394 | 1.00 38.57 |
| MOTA | 5836 | CB | ASP B 353 | | 67.852 | | | |
| MOTA | 5837 | CG | ASP B 353 | | 67.134 | 9.986 | 78.315 | 1.00 43.90 |
| | | | ASP B 353 | | 66.034 | 9.851 | 78.926 | 1.00 22.39 |
| MOTA | 5838 | | | | 67.679 | 9.078 | 77.649 | 1.00 50.42 |
| MOTA | 5839 | OD2 | | | | | 77.202 | 1.00 35.83 |
| ATOM | 5840 | С | ASP B 353 | | 70.022 | 10.723 | | |
| - | 5841 | 0 | ASP B 353 | | 70.189 | 9.833 | 76.368 | 1.00 23.71 |
| ATOM | | N | PRO B 354 | | 70.954 | 11.025 | 78.116 | 1.00 36.36 |
| ATOM | 5842 | | | | 70.928 | 12.093 | 79.132 | 1.00 38.28 |
| ATOM | 5843 | CD | PRO B 354 | | | 10.277 | 78.212 | 1.00 33.62 |
| ATOM | 5844 | CA | PRO B 354 | • | 72.205 | | | 1.00 34.46 |
| ATOM | 5845 | CB | PRO B 354 | | 73.003 | 11.104 | 79.213 | |
| | 5846 | CG | PRO B 354 | | 71.896 | 11.556 | 80.164 | 1.00 38.08 |
| ATOM | | | PRO B 354 | | 71.924 | 8.883 | 78.733 | 1.00 33.62 |
| ATOM | 5847 | C | PRO B 354 | | 70.894 | 8.643 | 79.366 | 1.00 24.82 |
| MOTA | 5848 | 0 | PRO B 354 | | | 7.954 | 78.468 | 1.00 31.76 |
| MOTA | 5849 | N | TRP B 355 | | 72.833 | | | |
| ATOM | 5850 | CA | TRP B 355 | | 72.635 | 6.611 | 78.969 | |
| | | СВ | TRP B 355 | | 73.653 | 5.655 | 78.359 | 1.00 34.02 |
| MOTA | 5851 | | TRP B 355 | | 73.025 | 4.378 | 77.910 | 1.00 44.37 |
| MOTA | 5852 | CG | | | 73.263 | 3.072 | 78.436 | 1.00 45.39 |
| MOTA | 5853 | CD2 | | | | | 77.734 | 1.00 44.31 |
| ATOM | 5854 | CE2 | TRP B 355 | | 72.418 | | | |
| | 5855 | CE3 | TRP B 355 | | 74.107 | 2.569 | 79.432 | 1.00 47.19 |
| MOTA | | CD1 | | | 72.073 | 4.230 | 76.935 | 1.00 42.18 |
| MOTA | 5856 | | | | 71.704 | 2.910 | 76.826 | 1.00 37.84 |
| ATOM | 5857 | NE1 | | | | 0.808 | 77.999 | 1.00 44.97 |
| ATOM | 5858 | CZ2 | TRP B 355 | | 72.395 | | | 1.00 50.83 |
| ATOM | 5859 | CZ3 | TRP B 355 | | 74.084 | 1.207 | 79.694 | |
| | 5860 | CH2 | | | 73.231 | 0.341 | 78.979 | 1.00 48.73 |
| MOTA | | | TRP B 355 | | 72.819 | 6.685 | 80.485 | 1.00 30.67 |
| MOTA | 5861 | C | TRF 5 355 | | 73.622 | 7.474 | 80.981 | 1.00 26.93 |
| MOTA | 5862 | 0 | TRP B 355 | | | 5.880 | 81.218 | 1.00 24.96 |
| MOTA | 5863 | N | ARG B 356 | | 72.061 | | | |
| MOTA | 5864 | CA | ARG B:356 | | 72.147 | 5.848 | 82.671 | |
| | 5865 | CB | ARG B 356 | | 70.811 | 6:319 | 83.257 | 1.00 24.71 |
| MOTA | | | ARG B 356 | | 70.534 | 7.795 | 82.941 | 1.00 23.66 |
| MOTA | 5866 | CG | ARG 5 350 | | 69.067 | 8.212 | 83.055 | 1.00 20.14 |
| ATOM | 5867 | CD | ARG B 356 | | | | 82.642 | 1.00 20.59 |
| ATOM | 5868 | NE | ARG B 356 | | 68.926 | 9.610 | | 1.00 25.41 |
| ATOM | 5869 | CZ | ARG B 356 | | 67.787 | 10.192 | 82.288 | 1.00 23.41 |
| | 5870 | | 1 ARG B 356 | | 66.644 | 9.508 | 82.287 | 1.00 17.01 |
| atom | | NH | | | 67.796 | 11.464 | 81.910 | 1.00 20.07 |
| MOTA | 5871 | | | | 72.481 | 4.410 | 83.085 | 1.00 26.57 |
| ATOM | 5872 | C | ARG B 356 | | 71.610 | 3.641 | 83.485 | 1.00 23.02 |
| ATOM | 5873 | 0 | ARG B 356 | | | | 82.978 | 1.00 23.92 |
| ATOM | 5874 | N | GLY B 357 | | 73.761 | 4.063 | | 1.00 25.54 |
| ATOM | 5875 | CA | GLY B 357 | | 74.186 | 2.712 | 83.294 | |
| | 5876 | c | GLY B 357 | | 74.796 | 2.464 | 84.657 | 1.00 24.35 |
| ATOM | | | GLY B 357 | | 74.523 | 3.161 | 85.628 | 1.00 25.88 |
| ATOM | 5877 | 0 | GLI B 337 | | 75.638 | 1.444 | 84.718 | 1.00 24.32 |
| . ATCM | 5878 | N | GLY B 358 | | | 1.070 | 85.960 | 1.00 23.56 |
| ATOM | 5879 | CA | GLY B 358 | | 76.282 | | | 1.00 29.26 |
| ATCM | 5880 | С | GLY B 358 | | 76.412 | -0.441 | 85.924 | |
| | 5881 | ō | GLY B 358 | | 76.146 | -1.051 | 84.889 | 1.00 23.71 |
| ATOM | | | GLU B 359 | | 76.814 | | 87.033 | 1.00 27.64 |
| ATCM | 5882 | N | | | 76.955 | | 87.078 | 1.00 32.15 |
| ATOM | 5883 | CA | | | | | | 1.00 30.40 |
| ATOM | 5884 | CB | GLU B 359 | | 77.822 | | 88.265 | |
| | 5885 | | | | 77.125 | -2.772 | 89.601 | 1.00 31.23 |
| ATOM | | | | | 77.844 | -3.479 | 90.741 | 1.00 37.96 |
| ATOM | 5886 | | | | 77.287 | | | 1.00 33.89 |
| atcm | 5887 | | | | | | | |
| ATOM | 5888 | OE | 2 GLU B 359 | | 78.959 | | | |
| ATOM | 5889 | | GLU B 359 | | 75.571 | | | - |
| | | | GLU B 359 | | 74.612 | -2.429 | | |
| ATOM | 5890 | | VAL B 360 | | 75.482 | | 87.053 | 1.00 29.61 |
| ATOM | 5891 | | | | 74.230 | | | |
| ATCM | 5892 | . CA | | | | | | |
| ATOM | 5893 | C3 | | | 74.035 | | | |
| | 5894 | | 1 VAL B 360 | | 72.764 | -7.045 | | |
| ATOM | | | | | 73.969 | | | |
| ATOM | 5895 | | . AUT D 260 | | 74.342 | | | 1.00 26.00 |
| ATOM | 5896 | | VAL B 360 | | | | | |
| ATCM | 5897 | · 0 | VAL B 360 | | 75.150 | , -0.093 | | |

| | E000 |). NT | ARG | D | 361 | 73. | 553 | -5.289 | 89.575 | 1.00 | 26.45 |
|------|------|----------|-------|-----|-----|-----|---------|-----------|--------|------|--------|
| ATOM | 5898 | И | | | | 73 | 558 | -5.821 | 90.935 | 1.00 | 28.47 |
| ATOM | 5899 | CA | ARG | | | /3. | 220 | | 91.787 | | 30.55 |
| ATOM | 5900 | CB | ARG | В | 361 | | 479 | -5.146 | | | |
| | 5901 | CG | ARG | | 361 | 72. | 937 | -3.877 | 92.485 | | 32.61 |
| ATOM | | | | | 361 | 71 | 749 | -3.163 | 93.117 | 1.00 | 35.00 |
| MOTA | 5902 | CD | ARG | | | _ | 858 | -2.617 | 92.094 | | 30.31 |
| ATOM | 5903 | ΝE | ARG | | 361 | | | | | | 29.45 |
| MOTA | 5904 | CZ | ARG | В | 361 | | 753 | -1.925 | 92.350 | | |
| | 5905 | | ARG | | | 69. | 385 | -1.689 | 93.605 | 1.00 | 18.49 |
| MOTA | | 14117 | מות | 5 | 261 | | 041 | -1.428 | 91.348 | 1.00 | 30.49 |
| ATOM | 5906 | | ARG | в. | 307 | | | -7.322 | 91.001 | | 30.17 |
| MOTA | 5907 | С | ARG | | | | 351 | | | | |
| ATOM | 5908 | 0 | ARG | В | 361 | 72. | 665 | -7.910 | 90.168 | | 23.60 |
| | | | LYS | | 362 | 73 | 949 | -7.922 | 92.022 | 1.00 | 33.09 |
| MOTA | 5909 | N | | | | | 864 | -9.351 | 92.272 | 1.00 | 36.94 |
| MOTA | 5910 | CA | LYS | | | - | | | 93.513 | | 40.24 |
| MOTA | 5911 | CB | LYS | В | 362 | | . 687 | -9.706 | | | |
| ATOM | 5912 | CG | LYS | В | 362 | 76 | .190 | -9.527 | 93.337 | 1.00 | 52.55 |
| | 5913 | CD | LYS | | | 76 | . 571 | -8.126 | 92.849 | 1.00 | 56.65 |
| MOTA | | | | | | | .149 | -7.032 | 93.819 | 1.00 | 53.39 |
| MOTA | 5914 | CE | LYS | | 362 | | | | 93.341 | | 48.87 |
| ATOM | 5915 | NZ | LYS | | | | . 553 | -5.680 | | | |
| MOTA | 5916 | С | LYS | В | 362 | 72 | . 427 | -9.826 | 92.463 | | 32.84 |
| | | ō | LYS | B | 362 | 72 | .045 | -10.867 | 91.938 | 1.00 | 28.27 |
| ATOM | 5917 | | | | | | .628 | -9.075 | 93.215 | 1.00 | 34.67 |
| MOTA | 5918 | N | GLU | | | | | -9.493 | 93.435 | | 35.72 |
| MOTA | 5919 | CA | GLU | | | | . 245 | | | | |
| ATOM | 5920 | CB | GLU | В | 363 | 69 | .519 | -8.532 | 94.390 | | 36.04 |
| | | CG | GLU | | | 69 | .502 | -7.077 | 93.977 | | 44.81 |
| ATOM | 5921 | | | | 363 | | .859 | -6.186 | 95.033 | 1.00 | 52.14 |
| ATOM | 5922 | CD | GLU | | | | | -6.370 | 95.341 | | 48.46 |
| MOTA | 5923 | OE1 | | | 363 | | .661 | | | | |
| MOTA | 5924 | OE2 | GLU | В | 363 | 69 | .562 | -5.300 | 95.566 | | 57.31 |
| | 5925 | C | GLU | | | 69 | .501 | -9.619 | 92.111 | 1.00 | 30.68 |
| MOTA | | | | | | | | -10.530 | 91.944 | 1.00 | 30.45 |
| MOTA | 5926 | 0 | GLU | | | | | -8.724 | 91.166 | | 26.19 |
| ATOM | 5927 | N | VAL | В | 364 | | .784 | | | | |
| MOTA | 5928 | CA | VAL | В | 364 | 69 | .138 | -8.789 | 89.852 | | 24.65 |
| | 5929 | СВ | VAL | | | 69 | .536 | -7.599 | 88.958 | | 23.49 |
| MOTA | | | | | | | .924 | -7.770 | 87.563 | 1.00 | 21.01 |
| ATOM | 5930 | CG1 | | | | | | -6.293 | 89.587 | | 23.08 |
| MOTA | 5931 | CG2 | | | | | .049 | | | | |
| ATOM | 5932 | С | VAL | В | 364 | | | -10.083 | 89.144 | | 23.19 |
| | 5933 | ō | VAL | | 364 | 68 | .691 | -10.749 | 88.542 | | 23.06 |
| ATOM | | | | | 365 | 70 | 810 | -10.436 | 89.216 | 1.00 | 27.15 |
| ATOM | 5934 | N | | | | | | | 88.594 | 1 00 | 29.18 |
| ATOM | 5935 | CA | LYS | В | 365 | / 1 | | -11.000 | | | 28.61 |
| ATOM | 5936 | CB | LYS | В | 365 | | | -11.758 | 88.704 | | |
| ATOM | 5937 | CG | | | 365 | 73 | .554 | -10.617 | 88.030 | | 30.27 |
| | | | LYS | | 365 | 75 | .074 | -10.768 | 88.154 | 1.00 | 32.58 |
| ATOM | 5938 | CD | | | | | .790 | | 87.516 | 1.00 | 29.13 |
| MOTA | 5939 | CE | | | 365 | | | | 87.606 | | 35.17 |
| MOTA | 5940 | NZ | LYS | В | 365 | 77 | .271 | -9.689 | | | |
| ATOM | 5941 | С | LYS | В | 365 | 70 | | -12.879 | 89.276 | 1.00 | 25.30 |
| | 5942 | ō | | | 365 | 70 | .282 | -13.837 | 88.613 | | 26.81 |
| MOTA | | | | | | | | -12.831 | 90.604 | 1.00 | 26.10 |
| MOTA | 5943 | N | | | 366 | | | | 91.347 | | 28.29 |
| ATOM | 5944 | CA | ASP | В | 366 | 69 | 963 | -13.938 | | 1.00 | 20.23 |
| ATOM | 5945 | CB | ASP | В | 366 | 70 | .105 | -13.731 | 92.859 | 1.00 | 29.44 |
| | | | ACD | - B | 366 | 71 | . 557 | -13.669 | 93.311 | 1.00 | 32.95 |
| ATOM | 5946 | CG | | | | | | -14.099 | 92.551 | 1.00 | 26.37 |
| ATOM | 5947 | נסס | ASP | B | 300 | 72 | 011 | 12.035 | 94.442 | | 35.26 |
| MOTA | 5948 | OD2 | ASP | В | 366 | 71 | . SIT | -13.216 | - | | |
| | 5949 | С | ASP | В | 366 | 68 | .487 | -14.110 | 90.986 | 1.00 | 28.61 |
| MOTA | | | 100 | | 366 | 68 | 000 | -15.231 | 90.869 | 1.00 | 27.00 |
| MOTA | 5950 | 0 | | | | 65 | 777 | -13.002 | 90.801 | 1.00 | 28.63 |
| ATOM | 5951 | N | | | 367 | 0 / | . / / / | -13.002 | | 1 00 | 27.35 |
| ATOM | 5952 | CA | THR | В | 367 | 66 | .365 | -13.080 | 90.438 | 1.00 | , 2, |
| | 5953 | CB | THR | В | 367 | 65 | .726 | -11.683 | 90.359 | | 27.63 |
| ATCM | | | | | | 65 | 771 | -11.068 | 91.656 | | 28.12 |
| MOTA | 5954 | OG: | | | 367 | - 0 | 200 | -11.786 | | | 22.94 |
| MOTA | 5955 | CG | | | 367 | 64 | 280 | , -11./00 | | 1 00 | 25.46 |
| ATOM | 5956 | С | THR | В | 367 | 66 | 5.197 | -13.782 | 89.094 | | |
| | | | | | 367 | 65 | 3.389 | -14.693 | 88.964 | | 24.48 |
| ATOM | 5957 | 0 | | | | 6 | 962 | -13.361 | 88.092 | 1.00 | 23.33 |
| ATOM | 5958 | N | | | 368 | 0.0 | | 13.000 | 86.785 | | 28,.99 |
| ATOM | 5959 | CA | LEU | JB | 368 | 66 | .85/ | -13.990 | | | 77 67 |
| | 5960 | CB | | | 368 | 61 | 7.719 | -13.256 | 85.759 | | 27.67 |
| ATOM | | CG | | | 368 | 61 | 7.060 |) -12.070 | 85.046 | 1.00 | 29.47 |
| ATOM | 5961 | | | | | 21 | 5 007 | -12.607 | 84.195 | 1.00 | 32.45 |
| ATOM | 5962 | | 1 LEU | | | 0. | | _31 027 | | | 19.43 |
| ATOM | 5963 | CD: | 2 LEU | JB | 368 | 6 | . 546 | -11.027 | | | |
| | | | | | | | | | | | |

| | | | | | | 162 | -15.454 | 86.888 | 1.00 32.40 |
|--------|--------|------|-------|-------|-----|------------|---|---------|------------|
| ATOM | 5964 | С | | 368 | 67. | 202 | 15.300 | 86.179 | 1.00 31.80 |
| ATOM | 5965 | 0 | | 368 | | | -16.309 | | |
| | 5966 | N | GLU B | 369 | | | -15.735 | 87.774 | 1.00 33.59 |
| ATOM | 5967 | CA | | 369 | | | -17.101 | 88.003 | 1.00 39.68 |
| | 5968 | СВ | | 369 | 69. | 736 | -17.141 | 89.082 | 1.00 42.61 |
| ATOM | | | GLU B | | | | -17.138 | 88.537 | 1.00 50.65 |
| | 5969 | CG | | | | | -18.443 | 87.842 | 1.00 55.81 |
| MOTA | 5970 | CD | GLU B | 369 | | | | 87.299 | 1.00 57.42 |
| ATOM | 5971 | OE1 | GLU B | 369 | | | -18.561 | | 1.00 57.42 |
| MOTA | 5972 | OE2 | GLU B | 369 | | | -19.353 | 87.841 | |
| MOTA | 5973 | С | GLU B | 369 | 67. | 479 | -17.954 | 88.442 | 1.00 34.94 |
| | 5974 | ō | | 369 | 67. | 190 | -18.974 | 87.827 | 1.00 32.71 |
| MOTA | | | LYS B | | | | -17.541 | 89.512 | 1.00 34.92 |
| ATOM | 5975 | N | | | 65 | 656 | -18.295 | 89.993 | 1.00 35.12 |
| MOTA | 5976 | CA | | 370 | | | | 91.268 | 1.00 37.39 |
| MOTA | 5977 | CB | | 370 | 65. | 061 | -17.679 | | 1.00 44.70 |
| ATOM | 5978 | CG | LYS B | 370 | 65. | 879 | -17.916 | 92.532 | |
| ATOM | 5979 | CD | LYS B | 370 | | | -16.741 | 92.892 | 1.00 48.10 |
| | 5980 | CE | LYS B | 370 | 65. | 956 | -15.537 | 93.346 | 1.00 47.82 |
| ATOM | | NZ | LYS B | 370 | 66. | 804 | -14.387 | 93.786 | 1.00 45.41 |
| MOTA | 5981 | | | 370 | | | -18.375 | 88.930 | 1.00 33.21 |
| MOTA | 5982 | C | | | | | -19.409 | 88.773 | 1.00 29.52 |
| ATOM | 5983 | 0 | | 370 | 63. | 221 | 13.100 | 88.191 | 1.00 31.62 |
| ATOM | 5984 | N | | 371 | 64. | 390 | -17.288 | | 1.00 37.19 |
| ATOM | 5985 | CA | ALA B | 371 | 63. | 368 | -17.274 | 87.153 | |
| MOTA | 5986 | CB | | 371 | 63. | 392 | -15.938 | 86.403 | 1.00 35.65 |
| | 5987 | C | | 371 | 63. | 572 | -18.431 | 86.181 | 1.00 37.79 |
| MOTA | | | | 371 | 62 | 627 | -19.137 | 85.838 | 1.00 34.46 |
| ATOM | 5988 | 0 | | 372 | 64 | 810 | -18.644 | 85.759 | 1.00 40.10 |
| MOTA | 5989 | IJ | | | 04. | 1 47 | -19.698 | 84.792 | 1.00 40.46 |
| MOTA | 5990 | CA | LYS B | 372 | | | | 85.348 | 1.00 43.15 |
| MOTA | 5991 | С | | 372 | | | -21.066 | | 1.00 43.57 |
| ATOM | 5992 | 0 | LYS B | 372 | | | -22.053 | 84.591 | |
| ATOM | 5993 | CB | LYS B | 372 | | 654 | | 84.517 | 1.00 40.51 |
| | 5994 | CG | LYS B | | 67. | 029 | -18.925 | 83.248 | 1.00 20.00 |
| MOTA | | | LYS B | | | | -19.390 | 82.635 | 1.00 20.00 |
| MOTA | 5995 | CD | | | 60. | 511 | -20.907 | 82.706 | 1.00 20.00 |
| ATOM | 5996 | CE | LYS B | 3/2 | | | | 82.116 | 1.00 20.00 |
| MOTA | 5997 | NZ | LYS B | 372 - | 59. | 814 | -21:354 | | 1.00 47.80 |
| ATOM | 5998 | N | ALA B | | 64. | 412 | -21.159 | 86.624 | |
| MOTA | 5999 | CA | ALA B | 373 | 64. | 014 | -22.425 | 87.239 | 1.00 49.71 |
| | 6000 | CB | ALA B | 373 | 64. | 762 | -22.639 | 88.546 | 1.00 48.25 |
| ATOM | | c | | | 62. | 515 | -22.443 | 87.494 | 1.00 53.38 |
| ATOM | 6001 | | | 373 | | | | 86.903 | 1.00 58.01 |
| MOTA | 6002 | 0 | ALA B | | | 029 | | 88.269 | 1.00 55.13 |
| ATOM | 6003 | OXT | | 373 | | | | | 1.00 32.54 |
| HETATM | 2991 | ZN | en c | 1 | | 660 | | 109.464 | 1.00 28.76 |
| HETATM | 2992 | 31 | TSA D | 2 | | 669 | 8.189 | | 1.00 25.81 |
| HETATM | 2993 | 02 | TSA D | 2 | | 952 | | 108.340 | |
| HETATM | 2994 | 03 | TSA D | 2 | 52 | 458 | | 101.667 | 1.00 36.93 |
| TEIMIN | 2005 | N1 | TSA D | 2 | 47 | 800 | 7.789 | 108.131 | 1.00 31.21 |
| HETATM | | | | 2 | | 013 | | 101.259 | 1.00 30.57 |
| HETATM | | N2 | TSA D | | | 859 | | 101.610 | 1.00 28.47 |
| HETATM | 2997 | Cl | TSA D | 2 | | | | 101.666 | 1.00 25.57 |
| HETATM | 2998 | C2 | TSA D | 2 | | . 907 | | 101.000 | 1.00 21.68 |
| HETATM | 2999 | C3 | TSA D | | | 241 | | 101.551 | 1.00 21.00 |
| HETATM | 3000 | C4 | TSA D | 2 | 52 | . 626 | 0.026 | 101.366 | 1.00 23.11 |
| HETATM | 2001 | C5 | TSA D | | 53 | . 589 | 1.080 | 101.303 | 1.00 25.02 |
| HETATM | 2001 | | | | | . 218 | | 101.418 | 1.00 29.24 |
| HETATM | 3002 | . C6 | TSA D | | | | | 101.734 | 1.00 32.98 |
| HETATM | 3003 | C7 | TSA D | | | . 572 | | 101.996 | 1.00 29.05 |
| HETATM | 1 3004 | C8 | TSA D | 2 | | .108 | | 101.330 | 1.00 28.13 |
| HETATM | 1 3005 | C9 | TSA D | 2 | | . 052 | 5.421 | 103.338 | 1.00 26.13 |
| HETATM | 1 3006 | C10 | TSA D | 2 | 49 | .060 | 5.357 | 104.279 | 1.00 25.99 |
| HETATM | 3007 | C11 | | _ | 49 | . 315 | 6.155 | 105.504 | 1.00 32.05 |
| HETATE | 1 700, | | TSA D | 2 | | . 515 | 6.184 | 106.595 | 1.00 27.37 |
| HETATM | | | | | | . 855 | | 107.756 | 1.00 29.02 |
| HETATM | 1 3009 | C13 | | | | | | | 1.00 30.21 |
| HETAT | 1 3010 | C14 | | | | . 680 | | 104.132 | 1.00 30.60 |
| HETAT | 4 3011 | C15 | TSA D | 2 | | .776 | | 104.132 | 1.00 23.45 |
| HETATE | 4 3012 | C17 | | | | . 438 | | 101.139 | |
| HETAT | 1 3012 | C16 | | | 52 | .044 | -2.416 | 101.316 | |
| neTAT: | * 2004 | ZN | ZN E | _ | | . 949 | | 85.681 | 1.00 28.19 |
| HETATI | 4 0004 | | | _ | | .964 | | 85.428 | |
| HETAT | 4 6005 | 01 | TSA F | | | | | | |
| HETAT | M 6006 | 02 | TSA F | 2 | 21 | . 255 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | |

| нетатм | 6007 | 03 | TSA | F | 2 | | 51. | 569 | 6.5 | 12 | 93.2 | | | 27.89 |
|--------|--------|------|------------|------|----|---|-----|-------|------|--------------------|------|-------|------|---------|
| HETATM | 6008 | N1 | TSA | | 2 | | 50. | 347 | 1.2 | 221 | 86.6 | | | 27.23 |
| HETATM | 5000 | N2 | TSA | | 2 | | 47. | 061 | 11.1 | L39 | 93.7 | 13 | | 16.24 |
| HETAIM | 6010 | C1 | TSA | | 2 | | 49. | 443 | 7.5 | 79 | 93.3 | 04 | | 27.18 |
| HETATM | 6010 | C2 | TSA | | 2 | | 48. | 035 | 7.5 | 529 | 93.2 | 67 | | 25.98 |
| HETATM | POIT | | TSA | | 2 | | | 227 | 8.6 | | 93.3 | 98 | 1.00 | 24.59 |
| HETATM | 6012 | C3 | | | | | | 837 | | 71 | 93.5 | | | 25.75 |
| HETATM | 6013 | C4 . | TSA | | 2 | | | 274 | 10.0 | | 93.6 | | | 26.53 |
| HETATM | 6014 | C5 | TSA | | 2 | | | 041 | | 369 | 93.4 | | | 28.36 |
| HETATM | 6015 | C6 | TSA | | 2 | | | | | 105 | 93.1 | | | 25.27 |
| HETATM | 6016 | C7 | TSA | | 2 | | | 349 | _ | | 92.9 | | | 24.18 |
| HETATM | 6017 | C8 | TSA | | 2 | • | | 716 | | 006 | 91.5 | | | 27.20 |
| HETATM | 6018 | C9 | TSA | F | 2 | | _ | 134 | | 552 | | | | 30.21 |
| HETATM | 6019 | C10 | TSA | F | 2 | | | 419 | | 807 | 90.6 | | | _ |
| HETATM | 6020 | C11 | TSA | F | 2 | | | 118 | | 553 | 89.3 | | 1.00 | |
| HETATM | 6021 | C12 | TSA | F | 2 | | | 762 | | 624 | 88.4 | | | 23.47 |
| HETATM | 6022 | C13 | TSA | F | 2 | | 50. | 529 | | 462 | 87. | | | 28.28 |
| HETATM | 6023 | C14 | TSA | F | 2 | | 50. | 208 | | 019 | 93.9 | | | 28.83 |
| HETATM | 6024 | C15 | TSA | | 2 | | 48. | 013 | | 270 | 90. | | 1.00 | |
| HETATM | 6025 | | TSA | | 2 | | 47. | 699 | 12. | 456 | 93. | | | 27.37 |
| HETATM | 6025 | C16 | | | 2 | | 45. | 610 | 11. | 107 | 93. | | | 25.36 |
| HETATM | 6027 | OH2 | WAT | | 1 | | 61. | .391 | 6. | 723 | 88. | | 1.00 | 12.93 |
| HETATM | 6027 | | WAT | | 2 | | 55. | . 595 | -4. | | 83. | | 1.00 | 7.53 |
| HETATM | 6020 | OH2 | | | 3 | | 58. | 656 | 12. | 731 | 106. | 749 | 1.00 | 12.33 |
| HETATM | 6029 | OH2 | | | 4 | | | . 347 | 15. | 263 | 111. | 460 | 1.00 | 14.54 |
| HETATM | 6030 | OH2 | | | 5 | | | .523 | 13. | 627 | 76. | 224 | 1.00 | |
| HETATM | 6031 | OH2 | | | 6 | | | .466 | -6. | 064 | 85. | 688 | | 22.41 |
| HETATM | 6032 | | WAT | | 7 | | | | -17. | | 80. | 769 | | 21.99 |
| HETATM | 6033 | | | | 8 | | | .344 | -15. | 640 | 87. | 809 | 1.00 | 26.67 |
| HETATM | 6034 | OH2 | TAW TAW | | 9 | | | | -14. | | 83. | | 1.00 | 23.94 |
| HETATM | 6035 | | | | 10 | | | .540 | | | 122. | | 1.00 | 26.96 |
| HETATM | 6036 | | WAT | | | | | .414 | | 497 | 84. | | 1.00 | 22.51 |
| HETATM | 6037 | | WAT | | 11 | | | .671 | 18 | 074 | 114. | | 1.00 | 32.15 |
| HETATM | 6038 | OH2 | TAW | ٠ | 12 | | | .335 | 10 | 679 | 117. | 140 | | 19.47 |
| HETATM | 6039 | | WAT | | 13 | | | .565 | | 469 | | 366 | | 18.81 |
| HETATM | 6040 | | VAT | | 14 | | | .311 | | 237 | | 508 | | 26.11 |
| HETATM | 6041 | | TAW | | 15 | | | .628 | | 883 | 104. | | | 24.28 |
| HETATM | 6042 | | TAW | | 16 | | | | | 507 | | 576 | | 18.30 |
| HETATM | 6043 | OH2 | | | 17 | | | .672 | | 923 | | 709 | | 22.27 |
| HETATM | 6044 | OH2 | | | 18 | | | .830 | | 831 | 108. | | | 24.68 |
| HETATM | 6045 | OH2 | | | 19 | | _ | .813 | | | | 823 | | 30.00 |
| HETATM | 6046 | OH2 | raw ! | G | 20 | | | .885 | | 352 | | 841 | | 17.32 |
| HETATM | 6047 | OH2 | | | 21 | | 36 | .382 | | | | 422 | 1 00 | 27.38 |
| HETATM | 6048 | OH2 | NAT | G | 22 | | | | -10. | | | 346 | 1 00 | 21.73 |
| HETAT | 6049 | OH2 | LAW : | G | 23 | | | .802 | | 446 | 140. | | 1.00 | 34.17 |
| HETATI | 4 6050 | OH2 | CAW ! | G | 24 | | | .292 | | | | 744 | | 40.67 |
| HETAT | 4 6051 | OH2 | CAW S | G | 25 | | | .747 | | 830 | | | | 27.92 |
| HETAT | 4 6052 | OH2 | WAT | r G | 26 | | 41 | .952 | | . 19 | 100 | . 110 | 1.00 | 24.31 |
| HETAT | 4 6053 | OH2 | CAW S | r G | 27 | | | .268 | | | 106 | | 1.00 | 30.93 |
| HETATI | 1 6054 | OH2 | WA! | r G | 28 | | | .342 | | .79. | | .076 | | 29.34 |
| HETATI | 6055 | OH | WA? | r G | 29 | | | .651 | | . 985 | | .845 | 1.00 | , 22.34 |
| нетат | 4 6056 | | WA? | | 30 | | 39 | .287 | | . 257 | | .623 | 1.00 | 22.61 |
| HETAT | 4 6057 | | WA! | | 31 | | | .221 | | . 462 | | .256 | 1.00 | 29.85 |
| neava. | 4 6058 | | WA | | 32 | | | .167 | | | 107 | | 1.00 | 36.40 |
| BETVII | M 6059 | | WA: | | 33 | | 64 | . 657 | -2 | . 682 | | . 225 | | 18.70 |
| UEIVII | M 6060 | | WA! | | 34 | | 44 | .059 | -2 | . 698 [.] | | . 805 | 1.00 | 30.02 |
| HETATI | M 6061 | | 'AW | | 35 | | 38 | .480 | | .763 | | .051 | 1.00 | 28.03 |
| HETAT | 4 6061 | | NA! | | 36 | | | .899 | | .654 | 112 | .976 | | 0 26.46 |
| HETATI | M 6062 | | WA' | | 37 | | | .092 | | .145 | 93 | .309 | | 0 22.31 |
| HETAT | M 6063 | | WA' | | 38 | | | .194 | -1 | .400 | 118 | .878 | 1.0 | 0 30.83 |
| HETAT | M 6064 | OH. | Z WA | | 39 | | | .400 | | .200 | | .379 | | 0.30.98 |
| HETAT | M 6065 | | 2 WA | | | | | 1.024 | | .540 | | .852 | 1.0 | 0 38.13 |
| HETAT | м 6066 | OH: | 2 WA | T. C | 40 | | | 6.65 | | .880 | | .402 | 1.0 | 0 29.24 |
| HETAT | м 6067 | | 2 WA | | 41 | | | 1.976 | | 499 | 109 | .692 | 1.0 | 0 46.34 |
| HETAT | м 6068 | | 2 WA | | 42 | | | 5.533 | | .511 | 94 | .759 | 1.0 | 0 23.13 |
| HETAT | м 6069 | | 2 WA | | 43 | | | L.448 | | .833 | | .306 | 1.0 | 0 27.0 |
| HETAT | M 6070 | OH | 2 WA | T G | 44 | | - |).578 | , 13 | 107 | 105 | .248 | 1.0 | 0 42.43 |
| HETAT | M 6071 | | 2 WA | | 45 | | | | | .936 | | .021 | | 0 38.9 |
| HETAT | M 6072 | OH | 2 WA | TG | 46 | | 53 | 3.938 | , -y | . ,,0 | | | | |
| | | | | | | | | | | | | | | |

| HETATM | 6073 | OH2 | WAT | G | 47 | | 38.45 | | -0.443 | 63.035 | 1.00 2 | |
|---------|--------|------|--------|-----|-----|---|-------|-----|---------|-----------|--------|-------|
| HEININ | 6074 | | MAT | | 48 | | 64.78 | 6 | 7.930 | 107.466 | 1.00 3 | |
| HETATM | 6074 | | | | 49 | | 50.82 | | 36.521 | 114.809 | 1.00 4 | 0.51 |
| HETATM | 6075 | | WAT | | | | 22 05 | ž. | -10.352 | 68.080 | 1.00 3 | |
| HETATM | 6076 | | WAT | | 50 | | 33.30 | | 14 221 | 86.007 | 1.00 3 | |
| HETATM | 6077 | | WAT | G | 51 | | | | -14.321 | 79.836 | 1.00 3 | |
| HETATM | 6078 | OH2 | WAT | G | 52 | | 63.27 | | 10.210 | | | |
| HETATM | 6079 | | WAT | G | 53 | | 59.26 | 3 | -12.096 | 94.306 | 1.00 2 | |
| MEIAIM | 6090 | | WAT | | 54 | | 46.04 | 1 | 10.641 | 76.561 | 1.00 2 | 7.97 |
| HETATM | 6060 | | TAW | | 55 | | | | -13.620 | 89.775 | 1.00 2 | 4.25 |
| HETATM | 908T | | | | | | 76.60 | | 0.622 | 89.097 | 1.00 2 | 9.19 |
| HETATM | 6082 | | TAW | | 56 | | | | | 79.089 | | 4.05 |
| HETATM | 6083 | OH2 | WAT | G | 57 | | 53.55 | | 6.439 | | | 5.02 |
| HETATM | 6084 | OH2 | WAT | G | 58 | | 71.30 |)1 | 11.026 | 83.310 | | |
| HETATM | 6085 | | TAW | G | 59 | • | 28.18 | 88 | -9.956 | 81.594 | | 3.21 |
| REIAIM | 6005 | | TAW | | 60 | | 53.08 | 14 | 20.992 | 98.483 | 1.00 2 | 7.64 |
| HETATM | 6000 | | WAT | | 61 | | 59.48 | | 8.630 | 93.423 | 1.00 3 | 0.30 |
| HETATM | 6087 | | | | | | 26.19 | - | -3.809 | 95.805 | 1.00 3 | 3.04 |
| HETATM | 6088 | | TAW | | 62 | | | | -0.121 | 89.620 | | 7.39 |
| HETATM | 6089 | | TAW | | 63 | | 26.09 | | -0.121 | | 1.00 2 | |
| HETATM | 6090 | OH2 | WAT | G | 64 | | 47.10 | | | 109.711 | | |
| HETATM | 6091 | | WAT | | 65 | | 23.27 | | 0.731 | 92.275 | 1.00 | |
| HETATM | 6002 | | VAT | | 66 | | 45.34 | 10 | -24.751 | 72.694 | 1.00 | |
| HETATM | 6092 | 0112 | TAW | Č | 67 | | 33.75 | | 16.234 | 111.676 | 1.00 | 34.63 |
| HETATM | 6093 | | | | 68 | | 52.83 | | | 126.276 | 1.00 4 | 17.11 |
| HETATM | 6094 | | WAT | | | | | | 16.953 | 111.099 | 1.00 2 | |
| HETATM | 6095 | | WAT | | 69 | | 50.21 | | | | | 24.95 |
| HETATM | 6096 | OH2 | WAT | G | 70 | | 44.79 | | 5.844 | | | |
| HETATM | 6097 | OH2 | WAT | G | 71 | | 49.53 | 17 | -18.731 | | 1.00 | |
| HETATM | 6098 | | WAT | | 72 | | 76.37 | 79 | 10.131 | | 1.00 | |
| TEIMIM | 6000 | | MAT | | 73 | | 30.23 | | -8.086 | 87.873 | 1.00 | |
| HETATM | 6100 | | WAT | | 74 | | 45.32 | | 12.061 | | 1.00 | 30.80 |
| HETATM | 6100 | | | | | | 72.88 | | 5.360 | | 1.00 | 29.04 |
| HETATM | 6101 | | WAT | | 75 | | 72.00 | 7.4 | -23.046 | | 1.00 | |
| HETATM | 6102 | OH2 | | | 76 | | | | -23.040 | 100.345 | 1.00 | |
| HETATM | 6103 | OH2 | WAT | G | 77 | | 40.6 | | | | | |
| HETATM | 6104 | OH2 | | G | 78 | | | | -19.477 | | 1.00 | |
| HETATM | 6105 | OH2 | | | 79 | | 46.4 | 80 | -6.539 | | 1.00 | |
| HETAIM | (105 | | WAT | | 80 | | 35.7 | | -12:230 | 81.646 | 1.00 | |
| HETATM | 6100 | | | | 81 | | 28.2 | | 8.745 | 121.961 | 1.00 | 41.15 |
| HETATM | 6107 | OH2 | | | | | 68.8 | | 3.154 | | 1.00 | |
| HETATM | 6108 | OH2 | | | 82 | | | | | | 1.00 | |
| HETATM | 6109 | OH2 | | | 83 | | | | -11.158 | | 1.00 | |
| HETATM | 6110 | OH2 | WAT | G | 84 | | 75.3 | | -1.773 | 92.264 | | |
| HETATM | 6111 | OH2 | | | 85 | | 46.9 | 57 | 12.230 | | 1.00 | |
| HETATM | 6112 | OH2 | _ | | 86 | | 63.7 | 89 | 9.551 | 64.329 | 1.00 | |
| HETATM | 0112 | | | | 87 | | 60.6 | | 21.185 | 72.215 | 1.00 | |
| HETATM | 6113 | OH2 | | | | | 56.5 | | 9.50 | | 1.00 | 31.10 |
| HETATM | 6114 | OH2 | | | 88 | | 26.3 | | -0.876 | | 1.00 | 29.70 |
| HETATM | 6115 | OH2 | | | 89. | | | | -16.583 | | 1.00 | 32.85 |
| HETATM | 6116 | OH2 | TAK | G | 90 | | 67.6 | | -10.50 | | 1.00 | 42.95 |
| HETATM | 6117 | OH2 | WAT | G | 91 | | 23.9 | 10 | 1.899 | 82.068 | | |
| HET; TM | 6118 | OH2 | WAT | G | 92 | | 50.0 | | 4.10 | 117.380 | 1.00 | 30.05 |
| HEAT IN | 6 6110 | OH2 | WAT | Ġ | 93 | | 26.7 | 74 | -9.492 | 83.952 | 1.00 | 43.59 |
| HET.IM | 0113 | | WAT | | 94 | | 42.7 | | -0.63 | 7 113.787 | | 40.17 |
| HETAIM | 1 5120 | | | | | | 57.9 | | 7 989 | 134.170 | | 47.82 |
| HETATM | 1 6121 | | TAK | | 95 | | | | -3 550 | 119.086 | | 36.62 |
| HETATM | 6122 | | WAT | | 96 | | 54.4 | | 13 (0) | 5 101.718 | | 41.62 |
| HETATM | 1 6123 | OH2 | WAT | , G | 97 | | 53.0 | 65 | 11.09 | 5 101./10 | | |
| HETAT | 6124 | | WAT | | 98 | | 58.2 | 86 | -23.64 | 68.207 | | 45.98 |
| HETAT | 1 6105 | OH2 | | | 99 | | 54.8 | 55 | -9.61 | 4 121.975 | | 34.57 |
| HETATE | 1 0177 | | | | | | 57.4 | | -3.35 | 2 57.145 | | 42.14 |
| HETATN | 1 6126 | OH2 | | | | | 63.5 | | | 3 123.667 | 1.00 | 33.87 |
| HETATN | 4 6127 | OH2 | | | | | 40.1 | 20 | | | 1.00 | 30.23 |
| HETAT | 4 6128 | OH | TAW S | G | 102 | | | | -23.14 | | 1 00 | 52.01 |
| HETATI | 4 6129 | OH2 | TAW S | | | | 62.8 | | 6.91 | - | | 36.29 |
| 22m2m | 4 6130 | OH | | | 104 | | 34.5 | 66 | | | | |
| ELALE. | 4 6131 | Un. | VAT | | | | 51.5 | | 20.86 | 9 67.459 | | 36.85 |
| ==TAT | 4 6131 | | NAT | | | | 28.1 | | | 0 129.379 | 1.00 | 42.87 |
| HETATI | M 6132 | OH. | . NAL | | 100 | | 40.7 | 182 | -11.45 | | 1.00 | 43.62 |
| HETAT | M 6133 | OH: | LAW 2 | G | 10/ | | | | | | 1.00 | 41.95 |
| HETATI | M 6134 | | raw s | | | | 44.7 | - / | -0.00 | - | | 35.71 |
| והלהבה | M 6135 | OH | CAN: S | rG | 109 | | | | -11.90 | 0 34.ULS | | 35.40 |
| | M 6136 | OH: | CAW S | r G | 110 | | 49.5 | | | 3 100.800 | | 55.30 |
| EE IAII | W 6127 | | 2 WAT | | | | 75.8 | 353 | | 0 124.536 | | 56.20 |
| HETAT | N 013/ | | 2 WAT | | | | 54.3 | 83 | | 0 136.095 | 1.00 | 36.40 |
| HETAT | M 6138 | OH. | νA'. | | 112 | | J-1 | | | - | | |
| | | | | | | | | | | | | |

| | | | | | | | 1 76 | 4 67 | 113 | 1.00 | 37 N1 |
|---------|--------|---------|----------|-----|-----|-------|------------------|--------|--|------|---------|
| HETATM | 6139 | OH2 WAT | G 1 | .13 | 33 | .114 | 1.76 | | | 1.00 | |
| HETATM | | OH2 WAT | G 1 | .14 | 42 | .618 | | 7 102 | | | |
| | | OH2 WAT | | | 53 | .605 | -10.81 | .6 66 | .281 | 1.00 | |
| HETATM | | | | | | .410 | -1.01 | 0 90 | .400 | 1.00 | 34.72 |
| HETATM | 6142 | OH2 WAT | | | 60 | 000 | 3 78 | 9 110 | . 221 | 1.00 | 35.69 |
| HETATM | 6143 | OH2 WAT | | | | | | 9 112 | 425 | 1.00 | |
| HETATM | 6144 | OH2 WAT | G 1 | .18 | | .474 | 19.15 | 9 112 | . 423 | | |
| HETATM | 67.45 | OH2 WAT | | | 39 | .749 | -0.61 | 6 132 | .45/ | 1.00 | |
| HEIAIM | 6145 | OH2 WAT | | | | .921 | 1.08 | 39 137 | .137 | 1.00 | |
| HETATM | 6146 | | | | | .081 | 7.61 | | .105 | 1.00 | 40.86 |
| HETATM | 6147 | OH2 WAT | | | | | 12.01 | 7 105 | | | 33.58 |
| HETATM | 6148 | OH2 WAT | | | 35 | .554 | | | | | 38.10 |
| HETATM | | OH2 WAT | G 1 | L23 | 41 | .381 | -23.53 | | . 872 | | |
| TEIAIN | 6150 | OH2 WAT | G 1 | 24 | 31 | .999 | 1.99 | | .813 | | 33.97 |
| HETATM | 6130 | OH2 WAT | C 1 | 25 | | .761 | 10.28 | 35 101 | .654 | 1.00 | 47.66 |
| HETATM | 912T | | | | | .596 | | 54 133 | 642 | 1.00 | 37.98 |
| HETATM | 6152 | OH2 WAT | | | 30 | | 5 3/ | 17 136 | 114 | | 46.39 |
| HETATM | 6153 | OH2 WAT | G I | L27 | 59 | . 611 | 5.34 | 1 130 | . 114 | | 30.77 |
| HETATM | 6154 | OH2 WAT | G 1 | 128 | 24 | .190 | | 20 124 | .0/9 | | |
| HETATM | 6155 | OH2 WAT | G 1 | 129 | 70 | .078 | 4.45 | 55 86 | .283 | | 36.11 |
| HETATM | 6155 | OH2 WAT | 6 1 | 130 | 57 | .882 | -4.33 | 14 125 | . 597 | | 41.40 |
| HETATM | 9120 | UNZ WAI | 9 3 | 130 | 45 | 838 | -20.69 | | .884 | 1.00 | 35.98 |
| HETATM | 6157 | OH2 WAT | G. | 131 | 4.5 | .030 | 20.0. | 86 79 | | | 36.67 |
| HETATM | 6158 | OH2 WAT | G : | 132 | 4.7 | .5/4 | 3.10 | 00 /3 | 205 | | 45.40 |
| HETATM | 6159 | OH2 WAT | G : | 133 | | | -18.9 | OT 65 | .295 | | |
| HETATM | 6160 | OH2 WAT | G ' | 134 | 4.0 | .164 | 5.04 | 47 95 | .358 | | 31.38 |
| HETAIM | 0100 | OH2 WAT | ~ | 135 | | .268 | | 05 122 | .461 | | 38.16 |
| HETATM | PTPT | OHZ WAI | <u>.</u> | 133 | = . | 200 | -20.1 | | .212 | 1.00 | 37.55 |
| HETATM | 6162 | OH2 WAT | G. | 136 | 24 | 475 | 10 5 | 34 103 | | | 37.96 |
| HETATM | 6163 | OH2 WAT | G | 137 | 4: | .435 | -10.5 | 34 IO2 | 400 | | 43.94 |
| HETATM | 6164 | OH2 WAT | G | 138 | 31 | 633 | 25.0 | 30 106 | . 433 | | |
| HETATM | 61'65 | OH2 WAT | G | 139 | 79 | .029 | - 7.5 | | .606 | | 40.55 |
| REIAIM | 6165 | OH2 WAT | | | | 3.597 | 20.7 | 11 111 | 685 | | 33.25 |
| HETATM | 9100 | Onz WAI | | 141 | | .263 | 8.5 | 24 113 | 8.832 | 1.00 | 40.63 |
| HETATM | 6167 | OH2 WAT | | | 4.0 | 207 | -24 4 | 85 70 | 152 | 1.00 | 34.07 |
| HETATM | 6168 | OH2 WAT | G G | 143 | | | | | 3.604 | 1 00 | 32.22 |
| HETATM | 6169 | OH2 WAT | Ġ | 144 | | 3.383 | -3.8 | | | 1.00 | 35.94 |
| HETATM | 6170 | OH2 WAT | ' G | 145 | 42 | 2.360 | -0.7 | | 1.686 | 1.00 | 35.34 |
| DEIAIN | 6171 | OH2 WAT | · G | 146 | 34 | 1.421 | -3.3 | | 5.685 | 1.00 | 35.42 |
| HETATM | 01/1 | | | | | 1.506 | 3.4 | 09 89 | 579 | | 39.86 |
| HETATM | 61/2 | OH2 WAT | | 147 | | 1.963 | 10.6 | | 1.806 | 1.00 | 31.12 |
| HETATM | 6173 | OH2 WAT | G | 148 | ٠. | . 200 | | | 5.769 | | 46.65 |
| HETATM | 6174 | OH2 WAT | G | 149 | | | -15.0 | 00. 30 | | 1.00 | 39.22 |
| HETATM | 6175 | OH2 WAT | G | 150 | | 4.695 | | 91 13 | | 1.00 | 39.22 |
| HETATM | 6176 | OH2 WAT | G | 151 | 4 | 0.348 | 1.3 | | 1.905 | 1.00 | 34.09 |
| HETAIM | (177 | OH2 WAT | | 152 | 6 | 6.912 | 17.6 | 66 12 | 7.489 | | 45.19 |
| HETATM | 01// | Onz WAI | | 152 | | 1.096 | 19.9 | 00 10 | 3.232 | 1.00 | 43.45 |
| HETATM | [6178 | OH2 WAT | . G | 155 | | B.074 | | | 0.175 | 1.00 | 28.86 |
| HETATM | 6179 | OH2 WAT | G | 154 | | | | | 9.003 | 1 00 | 41.15 |
| HETATM | 6180 | OH2 WAT | G | 155 | 6 | 3.586 | -1.0 | 374 7 | | | 40.92 |
| HETATM | 6181 | OH2 WAT | r G | 156 | | | -22.2 | | 8.415 | | |
| HETATM | 6192 | OH2 WAT | r G | 157 | 6 | 2.443 | 13.7 | | 9.547 | | 33.69 |
| HEIMIN | . (102 | OH2 WAS | rc | 158 | 5 | 8.832 | 9.7 | 798 10 | 1.311 | | 31.00 |
| HETATM | | ONZ WA | | 150 | | 7.701 | -5.5 | 28 11 | 9.322 | 1 00 | 45.00 |
| HETATI | 1 6184 | OH2 WAS | ! G | 133 | | 3.599 | | | 1.274 | 1 00 | 38.43 |
| HETAT | 1 6185 | OH2 WAT | r G | 160 | | | | 27 0 | | 1 00 | 51.83 |
| HETATN | 1 6186 | OH2 WA | r G | 161 | | 3.540 | | | 6.111 | 1 00 | 41.92 |
| HETAT | 6187 | OH2 WAY | rG | 162 | | 9.915 | | 318 11 | 0.8/3 | 1.00 | 91.72 |
| HETATI | 6199 | OH2 WA | r G | 163 | 5 | 1.265 | -8.2 | | 0.546 | 1.00 | 31.25 |
| HETAIR | 1 0100 | OH2 WA | | 164 | 5 | 8.109 | 7.0 | 024 9 | 8.294 | | 46.30 |
| HETATI | 1 6189 | UHZ WA | | 104 | | 6.553 | | | 4.179 | 1.00 | 37.53 |
| HETATI | 4 6190 | OH2 WA | r G | 165 | 4 | 6.333 | | | 2.515 | 1 00 | 43.91 |
| HETATI | 4 5191 | OH2 WA | | | | | -21.0 | | | | 43.13 |
| HETATI | M 6192 | OH2 WA | T G | 167 | | 7.146 | | 958 10 | | | |
| 115155 | M 6193 | OH2 WA | T G | 168 | 4 | 7.445 | -3.0 | | 4.746 | 1.00 | 27.99 |
| HETAII | 4 6193 | OH2 WA | | | | 5.193 | | 304 6 | 3.562 | 1.00 | 36.05 |
| HETATI | 4 6194 | UHZ WA | 1 0 | 103 | | 6.176 | | | 2.024 | 1.00 | 39.63 |
| HETATI | M 6195 | OH2 WA | T G | 170 | | | | | 0.886 | | 44.69 |
| HETAT | M 6196 | OH2 WA | T G | 171 | 7 | 0.527 | | | | | 51.41 |
| HETAT | M 6197 | OH2 WA | TG | 172 | 6 | 7.166 | | | 4.628 | | 53.49 |
| מבשעש | м 6198 | OH2 WA | | | 1 | 9.700 | | | 1.850 | | 2 22 42 |
| UEIVI | 4 6100 | OH2 WA | | 174 | | 5.875 | | | 37.176 | | 38.63 |
| HETAT | M 6199 | ORZ NA | . G | 175 | - | 1.874 | | 432 9 | 1.682 | | 40.08 |
| HETAT | M 6200 | OH2 WA | 1 G | 1/3 | 2 | 6.77 | -6. | | 1.530 | 1.0 | 32.57 |
| HETAT | M 6201 | OH2 WA | | | - | | | | 9.317 | | 0 29.83 |
| HETAT | м 6202 | OH2 WA | T G | 177 | | 3.224 | | | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | 0 47.28 |
| UETAT | м 6203 | OH2 WA | TG | 178 | | 9.606 | | - | 32.470 | 1.0 | 0 36 00 |
| TELLIA. | M 6204 | OH2 WA | | | | 2.81 | 11. | 799 | 8.957 | 1.0 | 0 36.09 |
| ne TAT | r 0.04 | ··· | - 0 | , | - | | | • | | | |

| HETATM | 6205 | OH2 | WAT G | 180 | 38. | 589 | 18.249 | 88.356 | 1.00 | |
|--|--------|------|---------|-------|------|--------|----------|-----------|------|---------------------|
| HETATM | 6206 | | WAT G | | 43. | 734 | -15.681 | 61.135 | 1.00 | |
| HETATM | 6200 | 0112 | WAT G | 182 | 42. | | 15.251 | 91.437 | 1.00 | 37.96 |
| HETATM | 6207 | | | | 57 | 121 | -11.129 | 126.206 | 1.00 | 45.78 |
| HETATM | 6208 | | WAT G | | 50 | 011 | -19.367 | 92.127 | 1.00 | |
| HETATM | 6209 | OH2 | WAT G | 184 | | | 2.453 | 95.969 | 1.00 | |
| HETATM | 6210 | | WAT G | | 56. | | 2.433 | | 1.00 | |
| HETATM | 6211 | OH2 | WAT G | 186 | 26. | | 14.125 | 125.052 | | |
| HETATM | 6212 | OH2 | WAT G | 187 | 24. | 631 | | 122.650 | 1.00 | |
| HETATM | 6213 | OH2 | WAT G | .188 | 23. | 516 | 4.964 | 81.599 | 1.00 | |
| HEIMIM | 6214 | OH2 | WAT G | 189 | 55. | 017 | 14.964 | 62.948 | 1.00 | |
| HETATM | 6214 | | WAT G | | | 371 | 13.710 | 105.640 | 1.00 | 37.04 |
| ${\tt HETATM}$ | 6215 | OHZ | WAIG | 100 | | | -10.386 | 91.144 | 1.00 | 36.62 |
| HETATM | 6216 | OHZ | WAT G | 191 | | 437 | 22 668 | 121.285 | | 38.19 |
| HETATM | 6217 | OH2 | WAT G | 192 | | | 24.057 | 122.112 | | 42.05 |
| HETATM | 6218 | OH2 | WAT G | 193 | | 786 | | 96.101 | | 48.35 |
| HETATM | 6219 | | WAT G | | | 852 | 3.461 | | | 32.60 |
| HETATM | 6220 | OH2 | WAT G | 195 | 41. | 681 | 11.318 | 92.011 | 1.00 | 47 70 |
| HETATM | 6221 | | WAT G | | 26. | 812 | -10.229 | 111.631 | 1.00 | 47.70 |
| HETATM | 6222 | OH2 | WAT G | 197 | 42. | 432 | -23.250 | 76.629 | | 48.86 |
| HETATM | 6223 | OH2 | WAT G | 198 | 25. | 484 | | 121.410 | | 43.09 |
| HETATM | 6223 | 0112 | WAT G | 199 | 43. | 514 | -20.514 | 111.706 | | 46.80 |
| HETATM | 5224 | 0112 | WAT G | 200 | 74 | 273 | -13.079 | 95.699 | 1.00 | 44.89 |
| HETATM | 6225 | OHZ | WATS | 200 | | 982 | 24 383 | 103.984 | 1.00 | 40.63 |
| HETATM | 6226 | OH2 | WAT G | 201 | | | -12.771 | 74.705 | | 35.13 |
| HETATM | 6227 | OH2 | WAT G | 202 | | | 9.211 | | | 33.53 |
| HETATM | 6228 | OH2 | WAT G | 203 | | 708 | | | | 48.49 |
| HETATM | 6229 | OH2 | WAT G | 204 | | 256 | | 122.243 | | 41.26 |
| HETATM | 6230 | OH2 | WAT G | 205 | | 706 | 16.208 | | | |
| HETATM | 6231 | OH2 | WAT G | 206 | 50. | 000 | 34.998 | | 1.00 | 39.15 |
| HETATM | 6232 | OH2 | WAT G | 207 | 68. | 078 | -16.236 | 83.621 | | 29.70 |
| HETATM | 5233 | OH2 | WAT G | 208 | 24. | 395 | -4.134 | 111.635 | | 50.82 |
| HEIAIM | 6233 | 0112 | WAT G | 209 | 53. | 384 | -2.664 | 114.289 | | 44.49 |
| HETATM | 6234 | 0112 | WAT | 210 | | 120 | | | | 31.97 |
| HETATM | 6235 | OHZ | WAT | . 210 | | 405 | | 111.744 | 1.00 | 44.97 |
| HETATM | 6236 | OH2 | WAT G | 211 | | .214 | | | | 59.14 |
| HETATM | | OH2 | WAT G | 212 | 30 | .754 | 6:983 | | | 41.78 |
| HETATM | 6238 | OH2 | WAT G | 213 | | | | | | 41.02 |
| HETATM | 6239 | OH2 | WAT G | 214 | | .820 | -0.465 | 1 22.101 | 1.00 | 38.42 |
| HETATM | 6240 | OH2 | WAT C | 215 | | .143 | 22.096 | 124.775 | 1.00 | 32.50 |
| HETATM | 6241 | OH2 | WAT | ; 216 | | .674 | | | 1.00 | 56.50 |
| HETATM | 6242 | он2 | WAT C | 217 | | .009 | | | | |
| HETATM | 6243 | OH2 | | 218 | 63 | .361 | | 109.653 | | 49.66 |
| HETATM | 6244 | OH2 | _ | 219 | 66 | .583 | -8.146 | | | 50.91 |
| HETATM | 6245 | OH2 | | 220 | 44 | .627 | -2.583 | | 1.00 | 36.99 |
| HEIMIN | 6 6245 | OH2 |) MAT (| 221 | 24 | .470 | -8.606 | | 1.00 | 47.24 |
| HETAT | | | WAT | | | .913 | | 83.973 | | 50.43 |
| HETAT | 1 624/ | | | 2 222 | | .788 | 0.651 | 129.136 | | 42.47 |
| HETAT | 1 6248 | OH2 | | | | | -16.880 | | 1.00 | 46.69 |
| HETAT | 1 6249 | | TAW S | | | .567 | | | | 43.17 |
| HETATI | 1 6250 | OH | WAT | 3 225 | | | | | | 35.84 |
| HETAT | 4 6251 | OH. | . WAT | 3 226 | | .681 | | | 1 00 | 42.39 |
| HETATI | 4 6252 | OH | TAW : | G 227 | | .263 | 15.23 | | | 52.23 |
| HETATI | 1 6253 | OH | 2 WAT | G 228 | _ | .933 | | 108.488 | | 46.56 |
| HETATI | 4 6254 | OH | XAT (| G 229 | 33 | .755 | 14.939 | 70.228 | | 1 40.30 |
| מבתאתו | 1 6255 | OH | WAT | G 230 | 51 | . 521 | | 4 100.859 | | 52.96 |
| TEINI- | 1 6256 | OH: | 2 WAT | G 231 | 34 | .140 | 0.56 | 5 63.039 | | 31.02 |
| HEIAII | 4 6255 | OH | 2 WAT | 332 | | .277 | | 7 81.662 | 1.00 | 39.83 |
| HETATI | 6257 | On | 2 WAT | C 233 | | .307 | | | 1.00 | 28.55 |
| HETATI | 4 6258 | | | | | .718 | | 0 125.707 | | 53.16 |
| HETAT! | 4 6259 | OH. | TAW S | G 234 | | . 624 | | | | 51.02 |
| HETAT | M 6260 | OH: | 2 WAT | G 235 | | | | | | 57.50 |
| HETAT | 4 6261 | OH: | 2 WAT | G 236 | | . 35.7 | | | | 38.65 |
| HETAT | M 6262 | | 2 WAT | | | .454 | | | _ | 44.95 |
| HETAT | M 6263 | OH: | 2 WAT | G 238 | | .836 | | | | 42.95 |
| הרהשת | M 6264 | OH | 2 WAT | G 239 | . 54 | . 933 | 3 23.34 | | _ | 0 45.78 |
| :::::::::::::::::::::::::::::::::::::: | M 6265 | ОН | 2 WAT | G 240 | 34 | | 2 -15.27 | | | U 41⊒./0 A 30 A1 |
| | M 5266 | | 2 WAT | G 241 | 35 | .966 | 6 -1.05 | | | 38.91 |
| ALIAI. | M 4247 | | 2 WAT | G 242 | 29 | . 681 | 7 1.89 | 8 127.376 | | 0 44.85 |
| HETAT | M 6267 | | 2 WAT | G 243 | 49 | .53 | 4 -10.15 | 0 113.501 | | 0 38.32 |
| HETAT | M 6268 | | 2 WAT | | | 7.25 | | 3 96.696 | 1.0 | 0 48.83 |
| HETAT | м 6269 | | | | | 2.31 | | | | 0 38.54 |
| HETAT | M 6270 | CH | 2 WAT | G 243 | 02 | | | • | | |
| | | | | | | | | | | |

| | | | | | | | | | | 7 00 | |
|-------------|--------|------|---------|---------|---|--------|-----|---------|-----------|------|-------|
| HETATM | 6271 | CH2 | WAT G | 246 | | 50.248 | | | 102.815 | 1.00 | |
| 11217111 | 6272 | OH2 | WAT G | 247 | | 47.966 | ; | 21.564 | 79.321 | 1.00 | 36.79 |
| HETATM | 62/2 | | | | | | | | 108.414 | 1.00 | 35 30 |
| HETATM | 6273 | OH2 | WAT G | 248 | | 62.507 | | | | | |
| HETATM | 6274 | OH2 | WAT G | 249 | | 53.971 | | 19.763 | 61.067 | 1.00 | |
| HEIAIM | 6076 | 0112 | WAT G | 250 | | 38.406 | | 9.828 | 67.749 | 1.00 | 33.71 |
| HETATM | 62/5 | | | | | | | | | 1.00 | |
| HETATM | 6276 | OH2 | WAT G | 251 | | 35.304 | | -6.179 | | | |
| HETATM | 6277 | OH2 | WAT G | 252 | | 39.218 | } - | 12.667 | 85.010 | 1.00 | 36.17 |
| HETATM | 02// | 0112 | WAI O | 252 | | 56.350 | | 5.089 | 97.225 | 1.00 | 46.38 |
| HETATM | 6278 | OH2 | WAT G | 253 | | | | | | | |
| HETATM | 6279 | OH2 | WAT G | 254 | | 69.850 |) | 3.406 | 122.119 | 1.00 | |
| 11517711 | 6380 | 0113 | WAT G | 255 | | 75.703 | } | 2.630 | 128.600 | 1.00 | 30.64 |
| HETATM | 6280 | | | | | 22 020 | ` | 12 973 | 113.965 | 1.00 | 34 48 |
| HETATM | 6281 | | WAT G | | - | | | | 113.303 | | |
| HETATM | 6282 | OH2 | WAT G | 257 | | 54.081 | Ĺ | 3.421 | 56.994 | | 39.11 |
| DEIRII | 6202 | OH2 | WAT G | | | 32.801 | L | -6.170 | 91.078 | 1.00 | 35.72 |
| HETATM | 6283 | | | | | 45.040 | | 0.301 | 95.449 | 1 00 | 36.57 |
| HETATM | 6284 | | WAT G | | | | | | | | 40.10 |
| HETATM | 6285 | OH2 | WAT G | 260 | | 39.815 | | | 128.855 | | |
| 11217111 | 6286 | OH2 | WAT G | 261 | | 28.763 | 3 | 10.408 | 93.790 | 1.00 | 44.39 |
| HETATM | 0200 | 0112 | C | 202 | | 40 669 | · _ | 12.050 | 60.539 | 1.00 | 50.89 |
| HETATM | 6287 | OH2 | WAT G | | | | | 12.030 | | | 62.67 |
| HETATM | 6288 | OH2 | WAT G | 263 | | 64.353 | | | 117.495 | | _ |
| 112222 | 6289 | | WAT G | | | 75.183 | 3 | 13.021 | 128.124 | 1.00 | 50.42 |
| HETATM | 0203 | | | | | | | 6.826 | 52.485 | 1.00 | 46.86 |
| HETATM | 6290 | он2 | | | | 46.289 | | | 70.958 | | 37.90 |
| HETATM | 6291 | OH2 | WAT G | 266 | | 68.708 | 3 | 13.973 | | | |
| 11513111 | 6202 | | WAT G | | | 71.504 | 4 | 12.997 | 130.029 | 1.00 | 38.78 |
| HETATM | 0232 | | | | | 36.309 | | -4 716 | 130.364 | 1.00 | 42.92 |
| HETATM | 6293 | | WAT G | | | | | | | | |
| HETATM | 6294 | OH2 | WAT G | 269 | | 65.973 | 3 | 12.195 | 79.625 | | 51.68 |
| III I MILI | 6205 | OH2 | | | | 71.952 | 2 | 13.021 | 74.292 | 1.00 | 37.70 |
| HETATM | 6295 | | | | | 44 433 | 2 | -17.578 | 62.734 | 1.00 | 49.33 |
| HETATM | 6296 | CH2 | | | | | | | | - | |
| HETATM | 6297 | OH2 | WAT G | 272 | | 26.91 | | 15.038 | 89.067 | | 38.07 |
| | 6200 | OH2 | | | | 63.380 | 0 | -5.416 | 126.550 | 1.00 | 41.73 |
| HETATM | 0230 | | | | | 63.360 | | -5.356 | 95.641 | 1.00 | 37.54 |
| HETATM | 6299 | OH2 | | | | 65.500 | _ | | | | 37.42 |
| HETATM | 6300 | OH2 | WAT G | 275 | | 65.94 | / - | -13.015 | 97.485 | | |
| HETATM | 6301 | OH2 | | | | 26.40 | 6 | 25.831 | 117.328 | | 48.37 |
| HETAIM | 0501 | | | | | 41 89 | ٦ - | -10.251 | 98.201 | 1.00 | 46.36 |
| HETATM | 6302 | | WAT G | | | | | 6 507 | 117.764 | | 49.87 |
| HETATM | 6303 | OH2 | WAT G | 278 | | 30.34 | | | | | |
| HETATM | 6304 | OH2 | WAT G | 279 . | | 45.13 | 5 | 32:419 | 111.056 | | 43.93 |
| HETAIN | 6304 | , | | | | 50.55 | | -1.365 | 120.511 | 1.00 | 54.02 |
| HETATM | | OH2 | | | | | | 12 652 | 105.130 | | 31.10 |
| HETATM | 6306 | OH2 | | | | 60.42 | | | | | |
| HETATM | 6307 | OH2 | WAT G | 282 | | 30.34 | 2 | 2.204 | | | 45.19 |
| REININ | | | | | | 60.35 | 8 | 15.921 | 127.736 | 1.00 | 33.17 |
| HETATM | 6300 | OH2 | | | | 64.19 | | 3.421 | | 1 00 | 45.81 |
| HETATM | 6309 | OH2 | | | | | | | | | 48.98 |
| HETATM | 6310 | OH2 | WAT G | 285 | | 45.46 | 8 | | 105.853 | | |
| HETATM | 6311 | OH2 | | | | 47.51 | 4 | 3.808 | 98.279 | 1.00 | 46.45 |
| HETATM | 1 0311 | | | | | 72.14 | | -6.345 | | 1.00 | 40.04 |
| HETATM | 1 6312 | OH2 | | | | | | | | | 43.62 |
| HETATM | 6313 | OH2 | WAT G | 288 | | 54.14 | | -5.100 | | | |
| HETATM | 6314 | OH2 | NAT G | 289 | | 48.98 | 2 | 13.297 | | | 46.98 |
| HEIRIE | 1 0314 | | | | | 41.17 | | 34.107 | 115.807 | 1.00 | 51.76 |
| HETATM | | | WAT G | | | | | | 104.170 | | 44.27 |
| HETATM | 6316 | | WAT G | | | 36.49 | | | | | |
| HETATM | 6317 | OHO | WAT G | 292 | • | 48.58 | 0 | 23.117 | 85.456 | | 40.96 |
| HEINII. | | | WAT G | | | 55.85 | | 22.934 | 98.099 | | 40.95 |
| HETATN | 1 0219 | | | | | 61.72 | | 11.077 | | | 41.21 |
| HETATM | 1 6319 | OH2 | WAT G | 294 | | 61.72 | U | | | 1.00 | 42 22 |
| HETATI | 1 6320 | OH | WAT G | 295 | | | | -18.552 | 114.112 | | 42.32 |
| "FIVIE | . 6323 | 0111 | WAT G | 206 | | 53.00 | | -6.305 | 129.052 | | 37.41 |
| HETATM | 1 6321 | Onz | WAIG | 230 | | | | 24.928 | | 1 00 | 48.09 |
| HETATI | 4 6322 | OH2 | WAT G | 297 | | 70.25 | | 24.920 | | | |
| HETATN | 4 6323 | OH | NAT G | 298 | | 77.49 | | | 130.507 | | 51.77 |
| NEIAIL | | 0111 | NAT G | 200 | | 32.23 | .3 | 12.182 | 83.028 | 1.00 | 53.51 |
| HETAT | 4 6324 | OH. | . AT C | 433 | | | | 12.878 | | | 46.49 |
| HETATN | 4 6325 | OH | NAT G | 300 | | 40.66 | | 12.070 | | | 48.51 |
| ער ביד אינו | 1 6326 | OH: | NAT G | 301 | | 50.97 | | | 114.597 | | |
| | 4 6333 | On | WAT G | 302 | | 54.23 | 6 | 3.817 | 92.196 | | 41.15 |
| HETATI | 4 6327 | OH. | LAL C | , ,,,,, | | 59.52 | | -1.343 | | | 36.71 |
| HETATI | 4 6328 | OH2 | 2 WAT C | 303 | | | | | | _ | 47.70 |
| מה קור מו | 6329 | OH: | TAW S | 304 | | 70.33 | 1 | 3.940 | | | |
| | 4 5330 | OH: | | | | 60.€2 | 6 | 6.969 | 127.780 | | 41.96 |
| HETATI | 4 6330 | UM. | | | | 42.15 | . 6 | -0.139 | | 1.00 | 32.19 |
| HETATI | 4 6331 | OH. | 2 WAT C | ە∪د , | | | | | | | 53.60 |
| | 4 6332 | OH: | 2 WAT C | 307 | | 58.88 | | 16.514 | | | |
| | 4 6333 | On. | 2 WAT | 308 | | 67.51 | 7 | -1.589 | | | 40.36 |
| EL AT | | O11. | | 300 | | 35 86 | 5.8 | -10.936 | | 1.00 | 48.80 |
| HETATI | 4 6334 | OH. | 2 WAT C | צטכ נ | | JJ.00 | 76 | 25 399 | 3 131.914 | | 48.99 |
| בייבייביי | 4 6335 | OH | 2 WAT C | 310 | | 45.57 | 0 | | | 1 00 | 27 06 |
| | M 6336 | CH | 2 WAT C | 311 | | 37.58 | 33 | -6.243 | 3 64.257 | 1.00 | 37.06 |
| HE LATE | 0330 | J.1. | / | | | - | | | • | | |
| | | | | | | | | | | | |

| | | | | | | | | | 1 00 45 07 |
|--|--------|------|------------|--------|---|--------|---------|-----------|------------|
| HETATM | 6337 | OH2 | WAT G | 312 | | 66.759 | 16.408 | 94.600 | 1.00 45.07 |
| HEINIH | 6336 | OH2 | MAT G | 217 | | 24.142 | 11.212 | 113.340 | 1.00 52.23 |
| HETATM | | | | | | 69.409 | 16.702 | 64.230 | 1.00 39.88 |
| HETATM | 6339 | OH2 | WAT G | 314 | | | 24 050 | 115.328 | 1.00 50.23 |
| HETATM | 6340 | OH2 | WAT G | 315 | | 22.064 | 24.858 | 113.326 | |
| HETATM | 6341 | OH2 | WAT G | 316 | | 50.171 | 9.551 | 100.345 | 1.00 37.32 |
| REIMIN | 6343 | 0112 | WAT G | 317 | | 55.104 | 31.302 | 119.497 | 1.00 44.78 |
| HETATM | 6342 | OHZ | WAT | 317 | | 65.333 | | 95.866 | 1.00 44.21 |
| HETATM | 6343 | OH2 | WAT G | | | | -10.103 | | 1.00 41.95 |
| HETATM | | OH2 | WAT G | 319 | | 31.415 | | 128.127 | |
| HETATM | 6345 | OH2 | | 320 | | 37.423 | 13.143 | 88.069 | 1.00 44.79 |
| HETATM | 6343 | | | 321 | | 43.619 | 14.292 | 96.509 | 1.00 54.69 |
| HETATM | 6346 | OHZ- | | | | | 14 555 | 126.016 | 1.00 42.75 |
| HETATM | 6347 | OH2 | WAT G | 322 | | 68.048 | | 120.010 | 1.00 37.06 |
| HETATM | 6348 | OH2 | WAT G | 323 | | 34.778 | -2.509 | 130.204 | 1.00 37.00 |
| HEITHIA | 6340 | OH2 | WAT G | 324 | • | 27.972 | 18.144 | 103.841 | 1.00 47.34 |
| HETATM | 0349 | | | | | 53.550 | 23.610 | 97.592 | 1.00 38.03 |
| HETATM | 6350 | OHZ | WAT G | 323 | | | 4.171 | 103.451 | 1.00 50.60 |
| HETATM | 6351 | OH2 | WAT G | 326 | | 33.776 | | | 1.00 48.34 |
| HETATM | 6352 | OH2 | WAT G | 327 | | 37.862 | 35.632 | 114.870 | |
| III I I I I I | 6353 | OH2 | WAT G | 328 | | 50.893 | 14.612 | 93.478 | 1.00 38.77 |
| HETATM | 6333 | 0112 | WAT G | 320 | | 71 422 | -20.913 | 86.137 | 1.00 47.69 |
| HETATM | 6354 | OHZ | WAT | 323 | | 50 310 | -23.133 | 74.502 | 1.00 41.94 |
| HETATM | 6355 | OH2 | WAT G | 330 | | | -23.133 | | 1.00 54.93 |
| HETATM | 6356 | OH2 | WAT G | 331 | | 41.520 | 7.269 | 60.583 | |
| HETATM | 6357 | OH2 | WAT G | 332 | | 75.879 | 13.737 | 106.089 | 1.00 44.65 |
| HETATM | 6357 | 0112 | WAT G | 333 | | 51.923 | 9.027 | 138.493 | 1.00 41.08 |
| HETATM | 6358 | OHZ | WAIG | 333 | | 49.511 | 27.611 | | 1.00 39.05 |
| HETATM | 6359 | | WAT G | | | | | 110.192 | 1.00 41.42 |
| HETATM | 6360 | OH2 | WAT G | 335 | | 69.385 | | | |
| HETATM | 6361 | OH2 | WAT G | 336 | | 40.952 | | 101.880 | 1.00 42.50 |
| REIAIM | (262 | 0112 | WAT G | 337 | | 32.998 | 7.200 | 103.784 | 1.00 54.22 |
| HETATM | 6364 | UNZ | WAIG | 227 | | 54.366 | 15 261 | 136.205 | 1.00 52.69 |
| HETATM | 6363 | | WAT G | | | | 13.727 | | 1.00 35.83 |
| HETATM | 6364 | OH2 | WAT G | 339 | | 35.674 | 13.727 | 03.132 | |
| HETATM | 6365 | OH2 | WAT G | 340 | | 66.606 | -21.361 | 87.138 | 1.00 46.26 |
| HETATM | 6366 | OH3 | WAT G | 341 | | 72.053 | 4.708 | 131.550 | 1.00 45.27 |
| HETATM | 6366 | 0112 | WAI C | ,343 | • | 28.072 | -1.358 | | 1.00 34.92 |
| HETATM | 6367 | | WAT G | | | | -3.981 | | 1.00 52.99 |
| HETATM | 6368 | | WAT G | | | 23.611 | -3.561 | 100.150 | 1.00 58.16 |
| HETATM | 6369 | OH2 | WAT G | 344 | | 53.684 | 2.564 | 122.150 | |
| HETATM | 6370 | OH2 | | | | 30.624 | -6:528 | 125.556 | 1.00 34.71 |
| HETAIR | 6370 | | | | | 27.870 | 13.838 | 113.997 | 1.00 44.91 |
| HETATM | 1 63/1 | | | | | 31.903 | -9 588 | 116.327 | 1.00 55.34 |
| HETATM | 1 6372 | | | | | 31.903 | | | 1.00 48.99 |
| HETATM | 6373 | OH2 | WAT G | 348 | | 71.763 | 15.094 | | |
| HETATM | 6374 | OH2 | WAT G | 349 | | 25.258 | | 114.760 | 1.00 37.19 |
| REIAIR | . (375 | OH2 | | | | 43.765 | 12.162 | 78.143 | 1.00 42.32 |
| HETATM | 1 03/3 | | | | | 32.452 | 5.338 | 73.909 | 1.00 33.70 |
| HETATM | 1 63/6 | OH2 | | | | 52.896 | | 101.894 | 1.00 46.40 |
| HETAT | 4 6377 | OH2 | | | | _ | | | 1.00 34.62 |
| HETATI | 4 6378 | OH2 | WAT G | 353 | | 47.968 | | 115.852 | 1.00 34.02 |
| HETATI | 4 6379 | OH2 | | | | 38.561 | -9.302 | | 1.00 49.80 |
| RETAIN | - 6300 | | | | | 63.791 | 17.454 | 74.354 | 1.00 56.40 |
| HETATI | 1 0300 | OH2 | WAIG | 355 | | 41.360 | 2 648 | 133.760 | 1.00 50.00 |
| HETAT | 4 6381 | | WAT G | | | | 7 035 | 122.328 | 1.00 38.01 |
| HETATI | 4 6382 | | WAT C | | | 42.467 | | | |
| וווע מידים | 4 6383 | OH2 | WAT G | 358 | | 50.890 | -0.362 | | 1.00 39.26 |
| 1151441 | 4 6384 | Uns | WAT G | 359 | | 54.217 | -23.881 | 67.865 | 1.00 55.18 |
| HETATI | 4 0304 | 0112 | | 360 | | 64.959 | 9.539 | 105.032 | 1.00 38.83 |
| HETAT | 4 6385 | OHZ | WAT C | 300 | | FO 113 | -19.846 | | 1.00 38.60 |
| HETATI | 4 6386 | OH2 | WAT | 361 | | | -19.040 | 02.500 | 1.00 31.47 |
| HELVAL | 4 6387 | OH2 | WAT C | 362 | | 42.245 | -1.140 | 93.572 | 1.00 51.47 |
| | 4 6388 | OH? | WAT C | 363 | | 73.552 | 17.770 | 125.885 | 1.00 54.89 |
| HETATI | . 6300 | 0112 | WAT | 361 | | 68.769 | 15.898 | 3 106.810 | 1.00 45.53 |
| HETATI | M 6389 | OHZ | WAT | 304 | | | | | 1.00 45.15 |
| HETATI | M 6390 | OH2 | WAT | 3 365 | | 37.543 | | | 1.00 44.99 |
| HETATI | M 6391 | OH2 | WAT | 366 | | 55.583 | | | 1.00 34.55 |
| 11222 | M 6392 | OH2 | TAK | 367 | | 41.284 | 9.699 | 9 78.250 | 1.00 36.58 |
| HEIAI | 0332 | 0112 | WAT | 368 | | 25.203 | | 2 126.362 | 1.00 46.60 |
| HETAT | M 6393 | OHZ | TAW | 3 300 | | 74.742 | | | 1.00 47.85 |
| HETAT | M 6394 | OH2 | TAW | 3 369 | | | | | 1.00 51.46 |
| HETAT | м 6395 | OH2 | WAT C | 370 | | 70.349 | | | |
| :::::::::::::::::::::::::::::::::::::: | м 6396 | OH2 | WAT (| 371 | | 42.936 | 20.63 | 1 94.720 | |
| SEIAI | | | WAT | 372 | | 34.162 | -16.11 | 4 114.141 | 1.00 44.01 |
| HETAT | M 5397 | | | 272 | | 33.863 | | 8 100.275 | 1.00 44.66 |
| HETAT | м 5398 | | TAW S | 3/3 | | | | | |
| HETAT | м 6399 | OH2 | TAW S | 374 | | 21.613 | 12.56 | | |
| 7547u | M 6400 | | TAW S | g 375 | | | | 2 100.583 | |
| ESIA! | M 5402 | | TAW S | 376 | | 70.095 | 13.39 | 5 117.505 | 1.00 52.02 |
| HETAT | M 5401 | | . 1625 L \ | 277 | | 41.853 | | 8 131.799 | 1.00 46.47 |
| HETAT | M 6402 | OH4 | TAW S | ١١ د د | | 41.000 | | • | |

| | | | | | | | | | 65.487 | . 00 | 49.09 |
|--|------------------|------|----------|-----|------|--------|------------|----------|---------------------|------|---|
| HETATM | 6403 | CH2 | WAT | G : | 378 | 55.780 | | | | | |
| HETATM | | OH2 | TAW | G. | 379 | 40.990 | | 1.205 | 91.611 | 1.00 | 41.02 |
| | | | | | | 48.157 | , , | 1 057 | 116.992 | 1.00 | 44.84 |
| HETATM | 6405 | | TAW | | | | | | 128.334 | | 37.09 |
| HETATM | 6406 | OH2 | WAT | G : | 381 | 37.954 | | 5.221 | | | |
| | | | TAW | | | 30.221 | . 2' | 7.743 | 109.194 | 1.00 | 39.92 |
| HETATM | | | | | | 49.926 | | | 118.421 | 1.00 | 58.95 |
| HETATM | 6408 | | WAT | | | 49.920 | -1 | 2.020 | | | _ |
| HETATM | | OH2 | WAT | G : | 384 | 42.435 | -1 | 7.636 | 81.477 | | 48.47 |
| | | | TAW | | | 58.226 | -2 | 5.990 | 71.378 | 1.00 | 48.18 |
| HETATM | | | | | | | | | 128.741 | | 43.82 |
| HETATM | 6411 | OH2 | WAT | G : | 386 | 40.495 |) <u>T</u> | | | | |
| HETATM | 6/12 | ೧೮೨ | WAT | G | 3.87 | 31.943 | | 6.301 | 109.475 | | 35.53 |
| | | | **** | ~ | 700 | 47.277 | , | 2.559 | 100.509 | 1.00 | 43.00 |
| HETATM | | | TAW | | | | | | 102.620 | | 31.70 |
| HETATM | 6414 | OH2 | WAT | G : | 389 | 38.862 | | 9.112 | | | |
| HETATM | 6/15 | OH2 | TAW | G | 390 | 71.652 | 2 1 | 4.568 | 105.167 | | 49.63 |
| | | 0112 | | ~ | 201 | 68.554 | | 0.518 | 73.331 | 1.00 | 38.16 |
| HETATM | | | TAW | | | | | | | | 32.16 |
| HETATM | 6417 | OH2 | TAW | G | 392 | 70.496 |) _T | p.100 | | | |
| HETATM | | 252 | WAT | G | 393 | 44.698 | 3 –2 | 4.950 | 75.603 | 1.00 | 43.38 |
| | | | | | | 56.172 | | 5.369 | | 1.00 | 47.44 |
| HETATM | 6419 | | WAT | | 394 | | | | | | 47.98 |
| HETATM | 6420 | CH2 | WAT | Ģ | 395 | 46.150 | | 9.441 | | | |
| | (401 | | WAT | | 396 | 26.892 | 2 - | 8.356 | 89.057 | | 34.99 |
| HETATM | | | | | | | | 4.380 | | : 00 | 50.78 |
| HETATM | 6422 | | WAT | | 397 | 31.73 | , . | 4.500 | 70.333 | | 50.86 |
| HETATM | 6423 | OH2 | WAT | G | 398 | 36.26 | l -1 | 3.824 | 62.777 | | |
| MEIAII | 6423 | | WAT | | 399 | 37.313 | 2 1 | 5,242 | 134.977 | 1.00 | 43.57 |
| HETATM | 6424 | | | | | 37.72 | | 2 773 | 126.419 | 1 00 | 57.13 |
| HETATM | 6425 | OH2 | WAT | G | 400 | 33.72 | | 2.113 | 120.312 | | |
| HETATM | | OH2 | WAT | G | 401 | 45.26 | | | 130.311 | | 49.55 |
| REIRIM | 6427 | | | ~ | 402 | 44.88 | 7 -1 | 7.414 | 111.508 | 1.00 | 54.29 |
| HETATM | 6421 | OH2 | | | | | | 0 455 | 136.711 | | 49.90 |
| HETATM | 6428 | | WAT | | | 68.92 | | | | | |
| HETATM | 6429 | OH2 | WAT | G | 404 | 43.27 | 1 -2 | 1.571 | 64.425 | | 48.61 |
| REIAIN | 6420 | | | | | 24.24 | ন – | 4.781 | 108.590 | 1.00 | 51.05 |
| HETATM | 6430 | OH2 | | | | | | 5.311 | | 7.00 | 43.43 |
| HETATM | 6431 | OH2 | | | | 54.82 | | | | | |
| HETATM | 6432 | OH2 | WAT | G | 407 | 53.46 | | | 124.076 | | 47.83 |
| | | 0112 | TAW | Č | 108 | 70.83 | 3 -1 | 8.390 | 85.386 | 1.00 | 49.26 |
| HETATM | 6433 | | | | | | | 5 297 | 113.071 | 1 00 | 34.52 |
| HETATM | 6434 | | WAT | | | 71.49 | / 1 | .3.407 | 113.071 | | |
| HETATM | 6435 | OH2 | TAW | G | 410 | 36.40 | 7 -1 | .8.480 | 110.466 | | 55.43 |
| REIAIM | 6436 | | | | | 26.22 | ი - | 9.551 | 78.158 | 1.00 | 47.69 |
| HETATM | 6436 | OH2 | | | | | - | 6.326 | | 1 00 | 42.00 |
| HETATM | 6437 | OH2 | | | 412 | 52.31 | | .0.320 | | | |
| HETATM | 6438 | OH2 | TAW S | G | 413 | 76.17 | 31 | .4.097 | 122.253 | | 44.90 |
| HETAIM | 6430 | | | | | 58.37 | | 6.335 | 123.024 | 1.00 | 54.61 |
| HETATM | 6439 | | TAW | | | | - - | 6.705 | | | 50.63 |
| HETATM | 6440 | OH2 | TAW S | G | 415 | 72.16 | | .0./0 | 02./13 | | |
| HETATM | 6441 | OH2 | | | | 63.55 | 7 2 | 26.152 | 65.944 | | 39.83 |
| HETATM | 0441 | | | | | 38.93 | | 3.070 | 122.742 | 1.00 | 52.57 |
| HETATM | 6442 | | TAW S | | | 55.55 | - 1 | 0 71 | 124.501 | 1 00 | 42.38 |
| HETATM | 6443 | OH2 | TAW S | G | 418 | | | 10.714 | 124.501 | | |
| HETATM | 6444 | 047 | TAW S | G | 419 | 55.44 | 3 - | -9.037 | 110.170 | | 46.47 |
| | | | | | | 73.87 | ٦ ، | 6.578 | 123.288 | 1.00 | 46.54 |
| HETATM | 1 6445 | OH2 | | | | | - | 2 66 | 117.527 | 1 00 | 43.62 |
| HETATM | 6446 | OH2 | | | 421 | 74.42 | | | | | |
| HETATM | 6117 | OHO | TAW S | G | 422 | 52.37 | 4 - | -0.368 | 3 51.502 | | 56.99 |
| DEIAIR | 1 0447 | | | | | 60.33 | 9 3 | 20.21 | 84.713 | 1.00 | 36.27 |
| HETATM | 1 6448 | | TAW S | | | | | 1.35 | | | 38.53 |
| HETATM | 6449 | OH2 | TAW S | G | 424 | 48.30 | | , | - 115 000 TOC.FC | | |
| HETATM | 6450 | OH: | 2 WAT | G | 425 | 61.75 | 7 2 | 21.60 | 5 115.976 | | 61.09 |
| BETAIR | | | , 1122 M | | 126 | 33 22 | 2 - | 14.91 | 119.528 | 1.00 | 51.12 |
| HETATM | 1 6451 | OH | Z WAT | ی | 420 | | | 2 25 | 112.298 | | 46.10 |
| HETATM | 4 6452 | OH | 2 WAT | G | 427 | 47.47 | | رود. د | , 114.430 | | |
| HETATM | 4 6453 | ua. | 2 WAT | G | 428 | 39.90 | 9 | 2.27 | 2 138.388 | | 35.33 |
| HETATE | 1 0433 | 0.11 | | . ~ | 420 | 57.82 | | 15.33 | 5 126.262 | 1.00 | 62.59 |
| HETATM | 1 6454 | CH. | 2 WAT | G | 429 | | | | 7 119.191 | 1 00 | 51.45 |
| HETATM | 4 6455 | CH: | 2 WAT | G | 430 | 48.91 | | -5.85 | , 113.131 | | |
| ************************************** | . 6166 | ΩÜ. | 2 WAT | | 431 | 44.13 | 9 . | -3.81 | 2 132.964 | 1.00 | 44.91 |
| HETATI | 1 0410 | 0112 | | . ~ | 422 | 38.88 | | 18.59 | 4 95.398 | 1.00 | 50.23 |
| HETAT | 1 6457 | OH | 2 WAT | ف | 434 | | | 7 00 | 4 55.271 | | 38.96 |
| HETAT | 4 6458 | OH: | 2 WAT | , C | 433 | 52.62 | | - / . 00 | | | 47 30 |
| | 4 5150 | | 2 WAT | · G | 434 | 60.64 | 4 | -0.73 | 1 101.129 | 1.00 | 47.30 |
| HETAT | 1 0433 | Jili | | . ~ | 12 E | 64.77 | | 5.80 | | 1.00 | 50.81 |
| HETAT | 4 6460 | OH: | 2 WAT | G | 433 | | | | | | 34.07 |
| HETAT: | 4 6467 | OH: | 2 WAT | G | 436 | 39.57 | | 16.70 | | | |
| | | 211 | 2 WAT | | 437 | 32.79 | 91 | -0.55 | 1 65.371 | | 41.40 |
| HETATI | | JH. | | | 120 | 58.33 | | -7 98 | 9 60.087 | 1.00 | 46.94 |
| HETAT: | 4 6463 | OH | 2 NAT | ં ઉ | 420 | | | · | 4 120 400 | | 46.28 |
| ಗಿದ್ದಿನಗು | M 6464 | ЭH | 2 WAT | G | 439 | 26.98 | | 5.4/ | 4 120.408 | 1.00 | 5 50 13 |
| ::E1WII | | 211 | 2 WAT | Ö | 440 | 72.13 | 8 8 | 1.23 | 3 90.050 | | 50.13 |
| HETATI | M 6465 | Un | A NAI | | 444 | 29.49 | | 10 97 | 1 118.393 | 1.00 | 56.30 |
| HETATI | M 6466 | ЭH | 2 WAT | : G | 441 | | | | 4 113.941 | | 58.17 |
| | | OH | 2 MATE | G | 442 | 69.2 | 52 | 5.59 | 4 113.241 | | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| | M KAKT | UR | | | | | | | | | _ /1 /7 |
| HETAT | M 6467 | | | | | 61.4 | 59 | 11.57 | 6 71.140 | 1.0 | 0 61.67 |
| HETAT | M 6467 M 6468 | | 2 WAT | | | 61.4 | 59 | 11.57 | 6 .71.140 | 1.0 | 0 61.67 |

| | | _ | | _ | | | 59.592 | 2.195 | 58.518 | 1 00 | 42.66 | |
|---------|------|-----|-----|----|-----|----|--------|---------|---------|------|-------|--|
| HETATM | 6469 | OH2 | TAW | G | 444 | | | | | | | |
| | | OH2 | TAU | G | 445 | | 47.407 | 6.152 | 111.310 | | 45.14 | |
| HETATM | | | | | | | 36.254 | 18.203 | 99.930 | 1.00 | 44.76 | |
| HETATM | 6471 | | TAW | | | | | | | | 47.72 | |
| MTATH | | OH2 | WAT | G | 447 | | 49.525 | 32.050 | 116.235 | | | |
| | | | | | | | 21.801 | -5.358 | 81.109 | 1.00 | 42.07 | |
| HETATM | 6473 | | TAW | | | | | | 95.380 | 1 00 | 40.76 | |
| HETATM | 6474 | OH2 | TAW | G | 449 | | 52.131 | -14.007 | | | | |
| | | | WAT | | | | 39 712 | -19.983 | 72.499 | 1.00 | 51.69 | |
| ·HETATM | | | | | | | | 5.620 | 67.102 | 1 00 | 42.38 | |
| HETATM | 6476 | OH2 | WAT | G | 451 | | 67.651 | | | | | |
| | | 043 | WAT | G | 452 | | 77.344 | 1.313 | 79.207 | | 63.64 | |
| HETATM | | | | | | | EE 240 | -29.426 | 86.187 | 1.00 | 44.98 | |
| HETATM | 6478 | OH2 | WAT | Ģ | 453 | | | | | 1 00 | 49.12 | |
| HETATM | | OH2 | WAT | G | 454 | | 64.429 | -11.004 | 98.104 | | | |
| | | | | | | | 45.456 | -0.814 | 129.510 | 1.00 | 61.60 | |
| HETATM | 6480 | | TAW | | | | | | 68.028 | 1 00 | 40.08 | |
| HETATM | | OH2 | WAT | G | 456 | | 65.066 | -14.790 | | | | |
| | | | WAT | | | | 34.732 | 5.611 | 94.924 | 1.00 | 58.32 | |
| HETATM | 6482 | ORZ | MWT | .5 | 40, | ٠, | 34 | • | | | | |

| Figure | 1 | 9- |] |
|--------|---|----|---|
|--------|---|----|---|

| | | | | D. | sidue | e il | X | Y | Z . | В | Segment | ID | |
|--------------|----------|----------|---------------|------|----------|---------|------------------|------------------|------------------|------|----------------------|----|------------------|
| | | CB | ALA | | 2 2 | u | 45.368 | 37.229 | 75.022 | | 57.10 | | بتبيية |
| ATCM | 1 | C = C | ALA | | 2 | | 46.761 | 38.761 | 73.244 | | 55.49 | | ببهجية |
| ATOM | 3 | S | ALA | | 2 | | 46.339 | 39.800 | 73.750 | 1.00 | 55.57 | | સેસેસ્સ |
| ATOM | د 4 | :: | ALA | | 2 | | 48.280 | 37.746 | 74.937 | | 57.26 | | ääää |
| ATOM | 5 | ca Ca | ALA | | 2 | | 47.062 | 37.537 | 74.110 | | 56.37 | | AAAA |
| ATOM | 5 | :: | LYS | | 3 | | | 38.628 | 71.938 | | 53.94 | | AAAA |
| ATOM | 7 | CÀ | LYS | | 3 | | 46.721 | 39.716 | 71.002 | | 51.97 | | AAA. |
| ATCH ATCM | . 8 | CE | | à | 3 | | 47.815 | 39.778 | 69.939 | | 53.86 | | AAAA |
| ATOM ATOM | 9 | CG | LIS | | 3 | | | .39.276 | 70.490 | 1.00 | 56.47 | | AAAA AAAA |
| ATOM | 10 | 22 | LYS | | 3 | | 50.252 | 39.570 | 69.387 | | 57.84 | | AAAA |
| ATOM | 11 | CE | LYS | | 3 | | 51.654 | 39.597 | 69.957 | 1.00 | 58.89 | | AAAA |
| ATOM | 12 | ::z | LYS | | 3 | | 52.643 | 39.283 | 68.895 | 1.00 | 59.33 | | AAAA |
| ATOM | 13 | c | LYS | À | 3 | | 45.393 | 39.494 | 70.305 | 1.00 | 49.57 49.33 | | AAAA |
| ATOM | 14 | Ō | LYS | | 3 | | 44.894 | 38.373 | 70.246 | | 46.23 | | AAAA |
| ATOM | 15 | 11 | VAL | A | · 4 | | 44.826 | 40.574 | 69.777 | | 42.51 | | AAAA |
| ATOM | 16 | CA | ::'AL | A | 4 | | 43.561 | 40.516 | 69.056 69.630 | | 42.26 | | AAAA |
| ATOM | 17 | CЗ | VAL | | 4 | | 42.543 | 41.516 | 68.940 | | 41.51 | | AAAA |
| ATCM | 18 | CG1 | VAL | A | 4 | | 41.213 | 41.352 | 71.128 | | 42.00 | | AAAA |
| ATOM | 19 | CG2 | VAL | A | 4 | | 42.401 | 41.307 | 67.638 | . 00 | 39.94 | | AAAA |
| ATOM | 20 | Ξ | VAL | | 7 | | 43.918 | 40.913 42.032 | 67.395 | 3 00 | 40.39 | | AAAA |
| ATOM | 21 | ਼ | VAL | | 4 | | 44.332 | 40.001 | 66.695 | | 36.94 | | AAAA |
| ATOM | 22 | :1 | LYS | | 5 | | 43.766 | 40.305 | 65.323 | | 34.10 | | AAAA |
| ATOM | 23 | CA | LYS | | 5 | | 44.142 45.179 | 39.290 | 64.846 | 1.00 | 35.02 | | AAAA |
| ATOM | 24 | CB | LYS | | 5 | | 46.424 | 39.182 | 65.698 | | 34.07 | | አልአል |
| ATOM | 25 | CG | LYS | À | 5 ' | | 47.233 | 40.452 | 65.652 | 1.00 | 33.44 | | ääää |
| ATOM | 26 | 22 | LYS | | 5 5 | | 48.555 | 40.239 | 66.333 | 1.00 | 32.38 | | ääää |
| ATOM | 27 | CE | LYS | - | 5 | | 49.372 | 41.460 | 66.222 | 1.00 | 31.26 | | aaaa |
| ATOM | 28 | ::2 | UYS UYS | ~ | 5 | | 42.997 | 40.293 | 64.333 | 1.00 | 31.38 | | AAAA |
| ATOM | 29 | C | LYS | | 5 | | 42.053 | 39.523 | 64.466 | 1.00 | 31.74 | | AAAA |
| ATOM | 30 | 0 17 | LEU | 2 | 6 | | 43.090 | 41.142 | 63.326 | 1.00 | 28.50 | | AAAA |
| ATOM | 31 | CA | LEU | Ξ. | 6 | | 42.075 | 41.167 | 62.289 | 1.00 | 26.90 | | AAAA |
| MOTA | 32 33 | CB | LEU | | 6 | | 41.530 | 42.580 | 62.067 | 1.00 | 26.43 | | AAAA |
| MOTA | 34 34 | cs | LEU | | 5 | | 40.321 | 42.748 | 61.129 | 1.0 | 25.89 | | aaaa aaaa |
| MOTA | 35 | . 551 | | | | | 40.108 | 44.224 | 60.826 | 1.0 | 0 25.50 | | AAAA |
| atom Atom | 36 | 200 | LEU | À | ร์ | | 40.550 | 42.032 | 59.828 | 1.0 | 0 26.64 | | AAAA |
| ATOM | 37 | | LEU | A | 5 | | 42.818 | 40.701 | 61.049 | 1.0 | 0 25.74 | | AAAA |
| ATOM | 38 | - | LEU | À | 5 | | 43.877 | 41.226 | 60.717 | 1.0 | 0 24.60 0 25.90 | | AAAA |
| ATOM | 39 | :: | ILE | A | 7 | | 42.282 | 39.704 | 60.367 | 1.0 | 0 26.75 | | AAAA |
| ATOM | 40 | | 112 | A | 7 | | 12.939 | 39.212 | 59.173 59.089 | 1.0 | | | አ እሕሕ |
| ATOM | 41 | 3 | === | À | ? | | 42.839 | 37.712 37.227 | 57.783 | 1.0 | | | AAAA |
| ATCM | 42 | 23 | 2 IL E | À | - | | 43.474 | | 60.310 | 1.0 | | | AAAA |
| ATCM | 43 | | 1 111 | À | Ξ | | 43.528 | 37.116 35.640 | 60.350 | | 0 27.46 | | አልልል |
| ATOM | 44 | CD | 1 ILE | : A | | | 43.507 | 39.814 | 57.929 | 1.0 | 0 25.70 | | AAAA |
| ATOM | 45 | | === | . A | <u>.</u> | | 42.339 41.162 | 39.655 | 57.581 | | 0 27.68 | | AAAA |
| ATOM | 46 | | === | | 7 | | 43.144 | 40.509 | 57.142 | | 0 27.94 | | AA A |
| atom | 47 | N | 323 | | 8 | | 42.598 | | | 1.0 | 0 29.78 | | AA/ A |
| ATOM | ÷8 | ÇA | GL | | 8 8 | | 43.587 | | | 1.0 | 0 30.38 | • | aaaa |
| ATOM | ÷9 | | | A | 8 | | 44.785 | | | 1.0 | 0 29.39 | | AAAA |
| ATOM | 50 | | | A : | 9 | | 43.051 | | 53.971 | 1.0 | 0 31.84 | | AAAA |
| ATOM | 51 | N CA | | 2 2 | 9 | | 43.832 | | 52.962 | | 0 32.41 | | AAAA |
| ATCM | 52 | | | 2 2 | 9 | | 44.606 | | 52.064 | | 0 31.12 | | AAAA |
| ATCM | 53 | | | | 9 | | 45.324 | | 51.053 | | 0 30.74 | | AAAA |
| ATOM | 54 55 | | | | 9 | | 43.654 | 41.140 | | | 0 30.27 | | AAAA |
| ATOM | 56 | | | R A | 9 | | 42.886 | | 52.091 | | 0 32.94 | | aaaa Aaaa |
| ATCM | 57 | | | R A | 9 | | 41.705 | 43.625 | | | 00 33.62 | | AAAA |
| ATOM | 56 | | | JÀ | 10 | | 43.396 | 45.009 | | | 00 33.20 | | 2444 2444 |
| ATOM | 59 | | | JA | 10 | | 42.573 | 45.840 | 50.611 | | 00 33.29 | | AAAA |
| ATOM | 50 | | | U A | | | 43.117 | 47.275 | 50.484 | | 00 33.12 | | - AAAA |
| ATOM ATOM | 5. | | | U A | | | 43.142 | | 51.566 | | 00 32.95 00 31.99 | | AAAA |
| ATOM | 5. 5. | | | U A | | | 41.743 | | 52.288 | | 00 34.71 | | AAAA |
| ATOM | 6. | | | U A | | | 44,116 | | 52.675 | | 00 33.18 | | AAAA |
| ATOM | 6 | | | ג ט | | | 42.527 | | 49.218 48.328 | | 00 32.52 | | AAAA |
| ATOM | 6 | | | IJ A | 10 | | 41.376 | | | 5 | 00 33.56 | | አአአአ |
| ATOM | 6 | | | P A | | | 43.230 | 44.12 | - 43.02 | ' | | | • |
| | | | | | | | | | | | | | |

| | | | | | | | | | | • |
|--------|-----|-----|--------|------|---|--------|------------------|---------|------------|--------|
| | | C. | ASP A | 11 | | 43.240 | 43.489 | 47.716 | 1.00 34.24 | AAAA |
| ATOM | 67 | | ASP A | 11 | | 44.393 | 42.499 | 47.607 | 1.00 35.81 | AAAA |
| MOTA | 68 | | | 11 | | 45.739 | 43.190 | 47.604 | 1.00 37.57 | AAAA |
| MOTA | 69 | | ASP A | | | 45.890 | 44.178 | 46.855 | 1.00 37.95 | AAAA |
| MOTA | 70 | | ASP A | 11 | | 46.650 | 42.750 | 48.332 | 1.00 40.31 | AAAA |
| MOTA | 71 | | ASP A | 11 | | 41.929 | 42.813 | 47.341 | 1.00 34.03 | AAAA |
| ATOM - | 72 | | ASP A | 11 | | | 42.652 | 46.150 | 1.00 34.80 | AAAA |
| ATOM | 73 | | ASP A | 11 | | 41.629 | | 48.335 | 1.00 32.34 | AAAA |
| ATOM | 74 | | TYR A | 12 | | 41.142 | 42.417 | 48.017 | 1.00 32.53 | AAAA |
| ATOM | 75 | CA | TYR A | 12 | | 39.871 | 41.803 | | 1.00 32.33 | AAAA |
| ATOM | 76 | CB | TYR A | 12 | | 39.043 | 41.569 | 49.290 | 1.00 31.32 | AAAA |
| ATOM | 77 | CG | TYR A | 12 | | 39.551 | 40.438 | 50.162 | | AAAA |
| ATOM | 78 | CD1 | TYR A. | 12 | | 39.983 | 40.669 | 51.469 | 1.00 28.52 | AAAA |
| ATOM | 79 | | TYR A | 12 | • | 40.413 | 39.614 | 52.279- | 1.00 28.03 | |
| ATOM | 80 | CD2 | TYR A | 12 | | 39.568 | 39.128 | 49.688 | 1.00 28.47 | AAA |
| ATOM | 81 | CE2 | TYR A | 12 | | 39.992 | 38.083 | 50.483 | 1.00 28.47 | AAAA |
| ATOM | 82 | CZ | TYR A | 12 | | 40.408 | 38.330 | 51.775 | 1.00 28.43 | - AAAA |
| | 83 | OH | TYR A | 12 | | 40.786 | 37.277 | 52.569 | 1.00 29.86 | AAAA |
| ATOM | 84 | c c | TYR A | 12 | | 39.146 | 42.749 | 47.066 | 1.00 33.16 | AAAA |
| MOTA | 85 | Õ | TYR A | 12 | | 38.554 | 42.324 | 46.082 | 1.00 33.36 | AAAA |
| MOTA | 86 | N | GLY A | 13 | | 39.237 | 44.041 | 47.356 | 1.00 34.76 | AAAA |
| ATOM | | CA | GLY A | 13 | | 38.594 | 45.065 | 46.546 | 1.00 36.60 | AAAA |
| MOTA | 87 | | GLY A | 13 | | 38.814 | 44.961 | 45.052 | 1.00 37.85 | AAAA |
| MOTA | 88 | C | GLY A | 13 | | 38.105 | 45.591 | 44.275 | 1.00 37.40 | AAAA |
| MOTA | 89 | 0 | LYS A | 14 | | 39.799 | 44.171 | 44.647 | 1.00 39.55 | AAAA |
| MOTA | 90 | N | LYS A | 14 | | 40.091 | 43.981 | 43.231 | 1.00 40.66 | AAAA |
| MOTA | 91 | CA | LYS A | 14 | | 41.605 | 43.977 | 42.995 | 1.00 42.26 | AAAA |
| MOTA | 92 | CB | | | | 42.300 | 45.309 | 43.239 | 1.00 44.54 | AAAA |
| ATOM | 93 | CG | LYS A | | | 41.820 | 46.445 | 42.304 | 1.00 46.32 | AAAA |
| ATOM | 94 | CD | LYS A | | | 42.033 | 46.158 | 40.810 | 1.00 46.64 | AAAA |
| ATOM | 95 | CE | LYS A | | | 41.133 | 45.086 | 40.256 | 1.00 47.23 | AAAA |
| MOTA | 96 | NZ | LYS A | | | 39.499 | 42.675 | 42.707 | 1.00 40.35 | AAAA |
| ATOM | 97 | C | LYS A | | | 39.593 | 42.377 | 41.511 | 1.00 39.97 | AAAA |
| ATOM | 98 | 0 | LYS A | | | 38.897 | 41.901 | 43.605 | 1.00 39.95 | AAAA |
| MOTA | 99 | N | TYR A | | | 38.300 | 40.617 | 43.245 | 1.00 40.30 | AAAA |
| ATOM | 100 | CA | TYR A | | • | | 39.490 | 44.050 | 1.00 38.46 | AAAA |
| MOTA | 101 | CB | TYR A | | | 38.962 | 39.519 | 44.021 | 1.00 37.01 | AAAA |
| MOTA | 102 | CG | TYR A | | | 40.472 | | 45.137 | 1.00 36.24 | AAAA |
| ATOM | 103 | CD1 | | | | 41.213 | 39.136 39.220 | 45.144 | 1.00 35.73 | AAAA |
| MOTA | 104 | CE1 | | | | 42.604 | | 42.902 | 1.00 36.84 | AAAA |
| MOTA | 105 | CD2 | TYR A | | | 41.163 | 39.976 | 42.898 | 1.00 36.53 | AAAA |
| MOTA | 106 | CE2 | | | | 42.556 | 40.064 | 44.028 | 1.00 36.24 | AAAA |
| MOTA | 107 | CZ | TYR A | | | 43.271 | 39.689 | | 1.00 36.49 | AAAA |
| ATOM | 108 | OH | TYR A | | | 44.648 | 39.816 | 44.042 | 1.00 41.98 | AAAA |
| ATOM | 109 | С | TYR A | | | 36.802 | 40.647 | 43.556 | 1.00 42.59 | AAAA |
| ATOM | 110 | 0 | TYR A | 15 | | 36.288 | 39.786 | 44.280 | 1.00 42.81 | AAAA |
| ATOM | 111 | N | ARG A | 16 | | 36.101 | 41.638 | 43.014 | 1.00 43.47 | AAAA |
| ATOM | 112 | CA | ARG A | 16 | | 34.670 | 41.753 | | 1.00 45.27 | AAAA |
| ATOM | 113 | CB | ARG A | 16 | | 34.205 | 43.197 | 43.111 | 1.00 48.06 | AAAA |
| ATOM | 114 | CG | ARG A | 16 | | 35.021 | 44.234 | | 1.00 49.63 | AAAA |
| ATOM | 115 | CD | ARG A | 16 | | 34.891 | 44.196 | | | AAAA |
| ATOM | 116 | NE | ARG A | 16 | | 35.632 | 45.322 | | | AAAA |
| ATOM | 117 | CZ | ARG A | | | 35.382 | 46.602 | | 1.00 52.71 | AAAA |
| ATOM | 118 | | ARG A | 16 | | 34.406 | 46.931 | | | AAAA |
| ATOM | 119 | | ARG A | | | 36.124 | 47.560 | | | AAAA |
| MOTA | 120 | С | ARG A | | | 33.913 | 40.929 | | | AAAA |
| ATOM | 121 | ō | ARG A | | | 34.455 | 40.541 | | | AAAA |
| | 122 | N | TYR A | | | 32.651 | 40.668 | | | |
| MOTA | 123 | CA | TYR | | | 31.818 | 39.942 | | | AAA |
| ATOM | 124 | | TYR | | | 30.675 | 39.254 | 42.333 | | AAAA |
| ATOM | | | TYR | - | | 31.097 | | | 1.00 38.35 | AAAA |
| MOTA | 125 | | TYR A | | | 32.169 | 38.148 | | 1.00 36.15 | AAAA |
| ATOM | 126 | | L TYR | 1 17 | | 32.519 | 37.069 | | 1.00 34.76 | AAAA |
| ATOM | 127 | _ | | _ | | 30:386 | | | 1.00 36.40 | AAAA |
| MOTA | 128 | _ | | - | | 30.726 | | 43.912 | 1.00 35.31 | AAAA |
| MOTA | 129 | | 2 TYR | | | 31.792 | | | 1.00 35.00 | AAAA |
| ATOM | 130 | | TYR . | | | 32.115 | | | 1.00 33.29 | AAAA |
| ATOM | 131 | | TYR . | | | 31.296 | | | 4 | AAAA |
| ATOM | 132 | C | TYR | A 17 | | 7 0 | | • | | • • |
| | | | | | | | • | | | |

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| | | | | | 1.8 | | | | |
|--------------|------------|---------|----------------|----------|------------------|------------------|------------------|--------------------------|----------------------------|
| - 2014 | 133 | 0 | TYR A | 17 | 31.346 | 42.194 | | 1.00 44.68 | AAAA |
| ATOM ATOM | 134 | | PRO A | 18 | 30.799 | 40.574 | •••• | 1.00 45.95 | AAAA AAAA |
| MOTA | 135 | | PRO A | 18 | 30.707 | 39.175 | 38.994 | 1.00 46.08 1.00 47.24 | AAAA |
| MOTA | 136 | CA | PRO A | 18 | 30.268 | 41.465 | 38.402 37.312 | 1.00 47.24 | AAAA |
| ATOM | 137 | | PRO A | 18 | 29.854 | 40.482 | 37.512 | 1.00 46.79 | AAAA |
| ATOM | 138 | | PRO A | 18 | 30.876 | 39.338 42.390 | 38.834 | 1.00 48.98 | AAAA |
| ATOM | 139 | | PRO A | 18 | 29.129 28.298 | 42.330 | 39.660 | 1.00 49.11 | AAAA |
| ATOM | 140 | | PRO A | 18 | 29.114 | 43.593 | 38.253 | 1.00 50.59 | AAAA |
| MOTA | 141 | | LYS A | 19 19 | 28.125 | 44.654 | 38.519 | 1.00 52.10 | AAAA |
| ATOM | 142 | | LYS A LYS A | 19 | 27.876 | 45.466 | 37.246 | 1.00 54.41 | AAAA |
| MOTA | 143 144 | | LYS A | 19 | 29.120 | 45.911 | 36.498 | 1.00 57.78 | AAAA |
| MOTA | 145 | | LYS A | 19 | 28.747 | 46.508 | 35.142 | 1.00 59.34 | AAAA AAAA |
| ATOM ATOM | 146 | | LYS A | 19 | 29.978 | 46.774 | 34.288 | 1.00 60.33 | AAAA |
| MOTA | 147 | | LYS A | 19 | 29.616 | 47.277 | 32.932 | 1.00 61.03 1.00 51.53 | AAAA |
| ATOM | 148 | С | LYS A | 19 | 26.764 | 44.162 | 39.012 40.071 | 1.00 51.55 | AAAA |
| ATOM | 149 | 0 | LYS A | | 26.281 | 44.556 43.314 | 38.203 | 1.00 50.13 | AAAA |
| ATOM | 150 | N | ASN A | | 26.146 24.831 | 42.750 | 38.482 | 1.00 48.44 | AAAA |
| MOTA | 151 | CA | ASN A | | 24.336 | 42.061 | 37.209 | 1.00 49.67 | AAAA |
| MOTA | 152 | CB | ASN A | | 25.389 | 41.132 | 36.613 | 1.00 51.61 | AAAA |
| MOTA | 153 154 | CG | ASN A | | 25.677 | 40.064 | 37.154 | 1.00 51.70 | AAAA |
| ATOM | 155 | ND2 | ASN A | | 25.998 | 41.562 | 35.509 | 1.00 53.00 | AAAA AAAA |
| ATOM ATOM | 156 | C | ASN A | | 24.789 | 41.765 | 39.649 | 1.00 45.57 1.00 44.67 | AAAA |
| ATOM | 157 | 0 | ASN A | | 23.764 | 41.127 | 39.877 40.398 | 1.00 42.71 | AAAA |
| ATOM | 158 | N | HIS A | | 25.883 | 41.662 | 41.506 | 1.00 40.69 | AAAA |
| ATOM | 159 | CA | HIS A | | 25.958 | 40.709 39.857 | 41.353 | 1.00 40.16 | AAAA |
| MOTA | 160 | СВ | HIS A | | 27.216 27.186 | 38.587 | 42.140 | 1.00 39.93 | AAAA |
| MOTA | 161 | CG | HIS A | | 27.329 | 38.353 | 43.467 | 1.00 39.27 | AAAA |
| ATOM | 162 | | HIS A | | 26.951 | 37.359 | 41.557 | 1.00 39.47 | AAAA |
| MOTA | 163 164 | | HIS 7 | | 26.948 | 36.425 | 42.493 | 1.00 39.36 | AAAA AAAA |
| ATOM ATOM | 165 | | HIS A | | 27.174 | 37.003 | 43.660 | 1.00 39.44 1.00 38.93 | AAAA |
| ATOM | 166 | C | HIS F | | 25.974 | 41.349 | 42.892 | 1.00 38.78 | AAAA |
| MOTA | 167 | 0 ' | HIS A | | 26.660 | 42.338 | 43.116 43.853 | 1.00 37.11 | AAAA |
| ATOM | 168 | N | PRO P | | 25.229 | 39.579 | 43.814 | 1.00 36.09 | AAAA |
| MOTA | 169 | CD | PRO A | | 24.371 25.224 | 41.361 | 45.199 | 1.00 35.81 | AAAA |
| ATOM | 170 | CA | PRO A | | 24.473 | 40.306 | 46.012 | 1.00 36.04 | AAAA |
| MOTA | 171 | CB | PRO A | | 23.464 | 39.810 | 45.003 | 1.00 36.19 | AAAA |
| MOTA | 172 173 | CG C | PRO A | | 26.638 | 41.637 | 45.751 | 1.00 34.39 | AAAA AAAA |
| MOTA ATOM | 174 | Ö | PRO A | | 26.867 | 42.653 | 46.417 | 1.00 34.09 | AAAA |
| ATOM | 175 | Ň | LEU | | 27.572 | 40.731 | 45.451 | 1.00 31.98 1.00 29.65 | AAAA |
| MOTA | 176 | CA | LEU | A 23 | 28.954 | 40.827 | 45.900 46.014 | 1.00 27.88 | AAAA |
| MOTA | 177 | CB | LEU 2 | | 29.564 | 39.432 38.528 | 47.048 | 1.00 27.31 | AAAA |
| ATOM | 178 | CG | LEU | | 28.896 29.656 | 37.217 | 47.149 | 1.00 26.64 | LAAA |
| ATOM | 179 | | LEU . | | 28.879 | 39.212 | 48.399 | 1.00 26.75 | AAAA . |
| MOTA | 180 | | LEU . | | 29.838 | 41.709 | 45.018 | 1.00 29.20 | AAAA |
| ATOM | 181 182 | C O | LEU | | 31.057 | 41.606 | 45.028 | 1.00 28.38 | AAAA |
| MOTA | 183 | N | LYS | | 29.204 | 42.582 | | 1.00 29.27 | AAAA AAAA |
| MOTA MOTA | 184 | | LYS | | 29.903 | 43.512 | | | AAAA |
| ATOM | 185 | | LYS | | 28.881 | 44.091 | | | AAAA |
| ATOM | 186 | CG | LYS | A 24 | 29.328 | | 41.601 41.994 | | AAAA |
| ATOM | 187 | | LYS | | 28.537 27.025 | | | | AAAA |
| MOTA | 188 | | LYS | | 26.221 | | | 1.00 34.37 | AAAA |
| ATOM | 189 | | LYS | | 30.580 | | | 1.00 28.14 | AAAA |
| ATOM | 190 | | LYS | | 31.617 | 45.162 | 43.840 | 1.00 27.93 | AAAA |
| MOTA | 191 | | LYS ILE | | 29.990 | 44.919 | 45.377 | | AAAA |
| MOTA | 192 193 | | | | 30.468 | 45.945 | 46.296 | | AAAA AAAA |
| MOTA MOTA | 194 | | | | 29.425 | 46.262 | 47.364 | | AAAA |
| atom | 195 | CG | 2 ILE | A 25 | 28.190 | 46.846 | | | AAAA |
| ATOM | 196 | CG | 1 ILE | A 25 | 01/ | | | | AAAA |
| ATOM | 197 | CD | 1 ILE | A 25 | | | | | AAAA |
| ATOM | 198 | 3 C | ILE | A 25 | 31.700 | , 40.00 | | = = | • |
| • | | | • | | | | | | |

| | | | | | J | | | | |
|--------------|------------|----------|----------------|----------|------------------|------------------|------------------|--------------------------|--------------|
| 3 mOM | 199 | o | ILE A | 25 | 32.037 | 44.379 | 47.183 | 1.00 24.48 | AAAA |
| ATOM ATOM | 200 | _ | PRO A | 26 | 32.375 | 46.547 | 47.714 | 1.00 24.98 | AAAA |
| MOTA | 201 | | PRO A | 26 | 32.062 | 47.980 | 47.638 | 1.00 24.98 | AAAA |
| ATOM | 202 | | PRO A | 26 | 33.570 | 46.367 | 48.543 | 1.00 24.44 | AAAA |
| ATOM | 203 | | PRO A | 26 | 34.094 | 47.792 | 48.701 | 1.00 24.75 | AAAA |
| MOTA | 204 | | PRO A | 26 | 33.435 | 48.546 | 47.538 | 1.00 25.51 | AAAA |
| ATOM | 205 | | PRO A | 26 | 33.021 | 45.838 | 49.862 | 1.00 23.42 | AAAA |
| ATOM | 206 | | PRO A | 26 | 31.930 | 46.233 | 50.272 | 1.00 22.12 | AAAA AAAA |
| ATOM | 207 | N | ARG A | 27 | 33.754 | 44.960 | 50.532 | 1.00 23.06 1.00 23.04 | AAAA |
| MOTA | 208 | | ARG A | 27 | 33.244 | 44.421 | 51.776 | 1.00 23.04 | AAAA |
| ATOM | 209 | | ARG A | 27 | 32.633 | 43.043 | 51.492 50.503 | 1.00 22.20 | AAAA |
| ATOM | 210 | | ARG A | | 31.463 | 43.152 | 50.303 | 1.00 19.64 | AAAA |
| MOTA | 211 | | ARG A | 27 | 30.762 | 41.844 41.168 | 51.315 | 1.00 16.51 | AAAA |
| MOTA | 212 | | ARG A | 27 | 30.181 30.774 | 40.188 | 51.982 | 1.00 16.57 | AAAA |
| MOTA | 213 | CZ | ARG A | 27 | 31.969 | 39.763 | 51.605 | 1.00 17.50 | AAAA |
| ATOM | 214 | | ARG A | 27 27 | 30.185 | 39.643 | 53.038 | 1.00 16.45 | AAAA |
| MOTA | 215 | | ARG A | 27 | 34.265 | 44.381 | 52.905 | 1.00 23.62 | AAAA |
| ATOM | 216 | C | ARG A | 27 | 34.107 | 45.077 | 53.919 | 1.00 23.69 | AAAA |
| ATOM | 217 | O N | ARG A VAL A | 28 | 35.305 | 43.570 | 52.736 | 1.00 24.25 | AAAA |
| MOTA | 218 219 | N CA | VAL A | 28 | 36.355 | 43.466 | 53.737 | 1.00 23.36 | AAAA |
| MOTA | 220 | CB | VAL A | 28 | 37.022 | 42.062 | 53.671 | 1.00 22.75 | AAAA |
| MOTA MOTA | 221 | | VAL A | 28 | 38.292 | 42.031 | 54.475 | 1.00 22.95 | AAAA |
| ATOM | 222 | | VAL A | 28 | 36.061 | 41.011 | 54.249 | 1.00 22.20 | AAAA |
| ATOM | 223 | c | VAL A | 28 | 37.363 | 44.609 | 53.511 | 1.00 23.70 | AAAA AAAA |
| ATOM | 224 | 0 | VAL A | 28 | 37.943 | 45.156 | 54.455 | 1.00 22.62 | AAAA |
| ATOM | 225 | N | SER A | 29 | 37.538 | 44.989 | 52.253 51.910 | 1.00 24.27 1.00 26.03 | AAAA |
| ATOM | 226 | CA | SER A | | 38.444 | 46.082 | 50.381 | 1.00 25.95 | AAAA |
| ATOM | 227 | CB | SER A | | 38.632 | 46.178 46.417 | 49.716 | 1.00 27.57 | AAAA |
| MOTA | 228 | og | SER A | | 37.395 37.793 | 47.354 | 52.440 | 1.00 25.52 | AAAA |
| MOTA | 229 | C | SER A | | 38.463 | 48.311 | 52.828 | 1.00 25.49 | AAAA |
| ATOM | 230 | 0 | SER A | | 36.468 | 47.342 | 52.448 | 1.00 26.09 | AAAA |
| MOTA | 231 | N | LEU A | | 35.692 | 48.471 | 52.926 | 1.00 26.39 | AAAA - |
| ATOM | 232 | CA CB | LEU A | | 34.262 | 48.365 | 52.393 | 1.00 25.89 | AAAA |
| ATOM | 233 234 | CG | LEU A | | 33.265 | 49.470 | 52.755 | 1.00 27.15 | AAAA |
| MOTA MOTA | 235 | | LEU A | | 32.486 | 49.101 | 53.999 | 1.00 26.34 | AAAA |
| MOTA | 236 | | LEU A | | 34.015 | 50.813 | 52.897 | 1.00 25.81 | AAAA |
| MOTA | 237 | c | LEU A | | 35.713 | 48.534 | 54.453 | 1.00 26.26 | AAAA AAAA |
| ATOM | 238 | 0 | LEU A | . 30 | 35.731 | 49.612 | 55.037 | 1.00 27.50 1.00 25.57 | AAAA |
| MOTA | 239 | N | LEU A | | 35.730 | 47.379 | 55.097 56.545 | 1.00 25.57 1.00 26.87 | AAAA |
| MOTA | 240 | CA | LEU A | | 35.776 | 47.343 | 57.029 | 1.00 27.28 | AAAA |
| MOTA | 241 | CB | LEU A | | 35.752 | 45.900 | 58.383 | 1.00 27.87 | AAAA |
| ATOM` | 242 | CG | LEU A | | 35.135 35.855 | 45.563 44.313 | 58.906 | 1.00 27.01 | AAAA |
| MOTA | 243 | | LEU A | | 35.855 35.261 | 46.706 | 59.372 | 1.00 26.32 | AAAA |
| MOTA | 244 | | LEU A | | 37087 | 48.003 | 57.012 | 1.00 28.08 | AAAA |
| ATOM | 245 | C | LEU A | | 37 094 | 48.854 | 57.901 | 1.00 27.42 | AAAA |
| MOTA | 246 | 0 N | LEU A | | 38.197 | 47.584 | 56.409 | 1.00 29.52 | AAAA |
| ATOM | 247 248 | N CA | LEU A | | 39.508 | 48.121 | 56.750 | 1.00 30.96 | AAAA |
| ATOM | 249 | CB | LEU A | - | 40.607 | 47.394 | 55.950 | 1.00 31.58 | AAAA |
| MOTA | 250 | CG | LEU A | | 40.792 | 45.904 | 56.293 | 1.00 31.63 | AAAA |
| MOTA MOTA | 251 | | LEU A | | 41.810 | 45.246 | 55.380 | 1.00 31.31 | AAAA |
| ATOM | 252 | CD2 | LEU A | 32 | 41.232 | 45.780 | 57.743 | 1.00 32.23 | AAAA |
| ATOM | 253 | c | LEU A | | 39.599 | | 56.543 | 1.00 31.59 | AAAA AAAA |
| ATOM | 254 | 0 | LEU A | | 40.081 | | | 1.00 31.70 1.00 32.72 | AAAA |
| ATOM | 255 | N | ARG A | | 39.140 | | | 1.00 32.72 | AAAA |
| ATOM | 256 | CA | ARG A | 33 | 39.178 | | | 1.00 35.10 | AAAA |
| ATOM | 257 | CB | ARG 2 | 33 | 38.643 | | | 1.00 37.84 | AAAA |
| ATOM | 258 | CG | ARG A | | 39.627 | | | | AAAA |
| ATCM | 259 | CD | ARG A | | 39.310 | | | | AAA |
| MOTA | 260 | NE | ARG | | 38.255 | | | | AAAA |
| MOTA | 261 | CZ | ARG : | A 33 | 37.662 38.016 | | | 1.00 44.61 | aaaa |
| MOTA | 262 | NH. | ARG | A 33 | 36.723 | | | 1.00 45.23 | AAAA |
| ATOM | 263 | | 2 ARG | | 38.352 | | | | AAAA |
| ATCM | 264 | С | ARG | A 33 | 30.332 | . ,,,,,,,, | • | | • |

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| | | | | • | 1 iguic 12 | • | | | |
|--------------|------------|----------|----------------|----------|------------------|------------------|------------------|--------------------------|-----------------------------|
| :2 EOM | 265 | 0 | ARG A | 33 | 38.713 | 53.390 | 56.592 | 1.00 33.61 | AAAA |
| MOTA MOTA | 266 | Ŋ | PHE A | 34 | 37.247 | 51.682 | 56.562 | 1.00 33.78 | AAAA |
| MOTA | 267 | CA | PHE A | 34 | 36.292 | 52.233 | 57.517 | 1.00 33.79 | AAAA |
| ATOM | 268 | CB | PHE A | 34 | 35.065 | 51.310 | 57.573 | 1.00 33.88 | AAAA |
| ATOM | 269 | CG | PHE A | 34 | 33.925 | 51.840 | 58.405 | 1.00 33.16 | AAAA |
| MOTA | 270 | | PHE A | 34 | 33.108 | 52.856 | 57.925 | 1.00 32.77 | AAAA |
| ATOM | 271 | | PHE A | 34 | 33.668 | 51.315 | 59.672 | 1.00 33.05 | AAAA |
| ATOM | 272 | | PHE A | 34 | 32.044 | 53.343 | 58.695 | 1.00 32.86 | AAAA |
| ATOM | 273 | CE2 | | 34 | 32.607 | 51.797 | 60.454 | 1.00 33.07 | AAAA |
| ATOM | 274 | CZ | PHE A | 34 | 31.794 | 52.809 | 59.966 | 1.00 32.58 | AAAA |
| ATOM | 275 | C | PHE A | 34 | 36.881 | 52.414 | 58.918 | 1.00 34.01 | AAAA |
| ATOM | 276 | O | PHE A | 34 | . 36.903 | 53.524 | 59.455 | 1.00 33.49 | AAAA |
| ATOM | 277 | N | LYS A | 35 | 37.350 | 51.324 | 59.516 | 1.00 34.00 | AAAA |
| ATOM | 278 | CA | LYS A | 35 | 37.928 | 51.401 | 60.843 | 1.00 33.90 | AAAA |
| MOTA | 279 | CB | LYS A | 35 | 38.230 | 50.010 | 61.362 | 1.00 34.07 | AAAA |
| ATOM | 280 | CG | LYS A | 35 | 37.000 | 49.190 | 61.662 | 1.00 33.94 | AAAA AAAA |
| ATOM | 281 | CD | LYS A | 35 | 37.414 | 47.810 | 62.106 | 1.00 35.31 1.00 35.91 | AAAA |
| ATOM | 282 | CE | LYS A | 35 | 38.062 | 47.072 | 60.948 | 1.00 35.91 | AAAA |
| ATOM | 283 | NZ | LYS A | 35 | 39.058 | 47.928 | 60.236 | 1.00 36.19 | AAAA |
| MOTA | 284 | С | LYS A | 35 | 39.185 | 52.255 | 60.881 61.929 | 1.00 34.19 | AAAA |
| MOTA | 285 | 0 | LYS A | 35 | 39.554 | 52.775 | 59.745 | 1.00 33.99 | AAAA |
| MOTA | 286 | N | ASP A | 36 | 39.853 | 52.384 53.216 | 59.680 | 1.00 35.17 | AAAA |
| MOTA | 287 | CA | ASP A | 36 | 41.034 | 52.943 | 58.388 | 1.00 37.40 | AAAA |
| MOTA | 288 | CB | ASP A | 36 | 41.812 | 53.908 | 58.186 | 1.00 38.64 | AAAA |
| ATOM | 289 | CG | ASP A | 36 | 42.964 43.648 | 54.218 | 59.184 | 1.00 40.02 | AAAA |
| MOTA | 290 | | ASP A | 36 | 43.201 | 54.341 | 57.035 | 1.00 38.74 | AAAA |
| MOTA | 291 | | ASP A | 36 | . 40.568 | 54.670 | 59.724 | 1.00 35.85 | AAAA |
| MOTA | 292 | C | ASP A | 36 36 | 41.231 | 55.527 | 60.306 | 1.00 36.88 | AAAA |
| MOTA | 293 | 0 | ASP A ALA A | 37 | 39.420 | 54.940 | 59.111 | 1.00 34.96 | AAAA |
| ATOM- | 294 | N CA | ALA A | 37 | 38.851 | 56.280 | 59.108 | 1.00 34.47 | AAAA |
| MOTA | 295 296 | CB | ALA A | 37 | 37.751 | 56.373 | 58.067 | 1.00 33.80 | AAAA |
| ATOM | 297 | C | ALA A | 37 | 38.291 | 56.617 | 60.499 | 1.00 34.66 | AAAA |
| MOTA MOTA | 298 | Ö | ALA A | 37 | 38.268 | 57.779 | 60.899 | 1.00 34.55 | AAAA |
| MOTA | 299 | N | MET A | 3.8 | 37.830 | 55.600 | 61.226 | 1.00 34.24 | AAAA |
| ATOM | 300 | CA | MET A | 38 | 37.287 | 55.794 | 62.572 | 1.00 33.07 | AAAA |
| ATOM | 301 | CB | MET A | 38 | 36.289 | 54.687 | 62.917 | 1.00 32.82 | AAAA |
| ATOM | 302 | CG | MET A | 38 | 35.084 | 54.559 | 61.996 | 1.00 32.72 | AAAA |
| ATOM | 303 | SD | MET A | 38 | 33.980 | 55.948 | 62.101 | 1.00 33.65 | AAAA AAAA |
| ATOM | 304 | CE | MET A | 38 | 33.550 | 55.878 | 63.849 | 1.00 33.77 1.00 33.12 | AAAA |
| ATOM | 305 | С | MET A | 38 | 38.430 | 55.724 | 63.583 | 1.00 33.12 | AAAA |
| ATOM | 306 | 0 | MET A | 38 | 38.226 | 55.930 | 64.777 | 1.00 32.64 | AAAA |
| MOTA | 307 | N | asn a | 39 | 39.628 | 55.428 | 63.090 63.935 | 1.00 32.38 | AAAA |
| ATOM | 308 | CA | ASN A | | 40.805 | 55.266 56.600 | 64.589 | 1.00 32.93 | AAAA |
| ATOM | 309 | CB | ASN A | | 41.200 | 57.736 | 63.571 | 1.00 34.40 | AAAA |
| MOTA | 310 | CG | ASN A | 39 | 41.393 42.180 | 57.624 | 62.630 | 1.00 34.98 | AAAA |
| MOTA | 311 | | L ASN A | 39 | 40.677 | 58.838 | 63.772 | 1.00 33.52 | AAAA |
| MOTA | 312 | | ASN A | 39 | 40.483 | 54.212 | 65.009 | 1.00 31.69 | AAAA |
| ATOM | 313 | C | ASN A | | 40.565 | 54.490 | 66.205 | 1.00 31.12 | AAAA |
| ATOM | 314 | 0 | ASN A | | 40.095 | 53.010 | 64.570 | | AAAA |
| ATOM | 315 | N | LEU A | | 39.750 | 51.898 | 65.474 | 1.00 32.48 | AAAA |
| MOTA | 316 | CA CB | LEU A | | 38.259 | 51.559 | 65.386 | 1.00 32.55 | AAAA |
| ATOM | 317 | CG | LEU A | | 37.231 | 52.581 | | 1.00 32.84 | AAAA |
| MOTA | .318 | | l LEU A | | 35.837 | 52.089 | 65.554 | 1.00 33.79 | AAAA |
| ATOM | 319 | | LEU A | | 37.372 | 52.798 | 67.376 | 1.00 32.45 | AAAA |
| MOTA | 320 321 | CD. | LEU A | | 40.555 | 50.628 | 65.187 | 1.00 32.92 | AAAA |
| ATOM | 322 | 0 | LEU A | | 40.196 | 49.530 | 65.618 | 1.00 31.64 | AAAA |
| MOTA | 323 | Ŋ | ILE A | | 41.652 | 50.794 | 64.464 | 1.00 34.12 | AAAA |
| ATOM ATOM | 324 | | ILE A | | 42.508 | 49.680 | 64.116 | 1.00 36.07 | AAAA |
| ATOM ATOM | 325 | | ILE A | | 42.017 | 48.991 | 62.811 | 1.00 35.51 | AAAA |
| ATOM | 326 | | 2 ILE A | | 42.070 | 49.952 | 61.636 | 1.00 33.37 | AAAA |
| ATOM | 327 | | l ILE A | | 42.898 | 47.790 | 62.480 | 1.00 35.97 | AAAA |
| ATOM | 328 | | 1 ILE A | | 42.854 | 46.701 | | 1.00 37.19 | AAAA AAA A |
| ATOM | 329 | | ILE A | | 43.921 | 50.226 | | 1.00 38.85 | AAAA |
| ATOM | 330 | | ILE A | | | 51.346 | 63.413 | 1.00 38.98 | WWW |
| | | | | | | | = | | • |

| | | | | | 0 | | | | |
|--------|-----|-----|-------|--------|--------|---|---------|------------|--------|
| | | ., | ASP A | 42 | 44.914 | 49.446 | 64.329 | 1.00 40.61 | AAAA |
| ATOM | | | | 42 | | 49.843 | 64.181 | 1.00 42.57 | AAAA |
| MOTA | | | ASP A | | 46.973 | 50.021 | 65.553 | 1.00 42.42 | AAAA |
| ATOM | | | ASP A | 42 | 46.316 | 51.110 | 66.381 | 1.00 42.27 | AAAA |
| MOTA | | | ASP A | 42 | | 52.250 | 65.883 | 1.00 41.20 | AAAA |
| ATOM | 335 | | ASP A | 42 | 46.227 | | 67.526 | 1.00 43.36 | AAAA |
| _MOTA | 336 | OD2 | ASP A | 42 | 45.891 | 50.833 | | 1.00 44.05 | AAAA |
| ATOM | 337 | С | ASP A | 42 | 47.011 | 48.752 | 63.392 | | AAAA |
| ATOM | - | 0 | ASP A | 42 | 46.525 | 47.620 | 63.333 | 1.00 44.88 | |
| ATOM | | N | GLU A | . 43 | 48.147 | 49.090 | 62.789 | 1.00 45.10 | AAAA |
| ATOM | | | GLU A | 43 | 48.905 | 48.141 | 61.980 | 1.00 46.11 | AAAA |
| | | | GLU A | 43 | 50.172 | 48.796 | 61.454 | 1.00 46.89 | AAAA |
| MOTA | | CG | GLU A | | 49.924 | 50.057 | 60.668 | 1.00 49.30 | AAAA |
| ATOM | | | GLU A | 43 | 51.187 | 50.580 | 60.028 | 1.00 49.67 | AAAA |
| ATOM | | CD | GLU A | | 51.760 | 49.839 | 59.201 | 1.00 50.60 | AAAA |
| MOTA | _ | | | | 51.601 | 51.714 | 60.349 | 1.00 49.60 | AAAA |
| . ATOM | | | GLU A | | 49.290 | 46.859 | 62.701 | 1.00 46.27 | - AAAA |
| MOTA | 346 | C | GLU A | | 49.214 | 45.773 | 62.131 | 1.00 46.00 | AAAA |
| MOTA | 347 | 0 | GLU A | | 49.708 | 46.986 | 63.954 | 1.00 46.52 | AAAA |
| ATOM | 348 | N | LYS A | | | 45.832 | 64.730 | 1.00 46.31 | AAAA |
| MOTA | 349 | CA | LYS A | | 50.135 | | 66.048 | 1.00 48.16 | AAAA |
| MOTA | 350 | CB | LYS A | | 50.762 | 46.306 47.215 | 65.799 | 1.00 51.59 | AAAA |
| ATOM | 351 | CG | LYS A | 44 | 51.977 | | | 1.00 52.87 | AAAA |
| ATOM | 352 | CD | LYS A | 44 | 52.641 | 47.734 | 67.071 | 1.00 53.34 | AAAA |
| ATOM | 353 | CE | LYS A | 44 | 53.851 | 48.601 | 66.727 | 1.00 53.34 | AAAA |
| ATOM | 354 | NZ | LYS A | 44 | 54.615 | 49.033 | 67.936 | | AAAA |
| ATOM | 355 | С | LYS A | | 49.029 | 44.828 | 64.996 | 1.00 44.74 | AAAA |
| ATOM | 356 | ō | LYS A | | 49.296 | 43.735 | 65.480 | 1.00 45.35 | |
| ATOM | 357 | N | GLU A | _ | 47.793 | 45.190 | 64.659 | 1.00 42.49 | AAAA |
| | 358 | CA | GLU A | | 46.638 | 44.320 | 64.894 | 1.00 40.54 | AAAA |
| ATOM | 359 | CB | GLU A | | 45.493 | 45.125 | 65.517 | 1.00 40.55 | AAAA |
| ATOM | | | GLU A | | 45.788 | 45.731 | 66.882 | 1.00 38.87 | AAAA |
| ATOM | 360 | CG | GLU A | | 44.663 | | 67.360 | 1.00 37.57 | AAAA |
| MOTA | 361 | CD | | | 44.383 | 47.631 | 66.693 | 1.00 36.29 | AAAA |
| ATOM | 362 | OE1 | | | 44.056 | 46.300 | 68.399 | 1.00 38.44 | AAAA |
| MOTA | 363 | OE2 | | | 46.126 | 43.648 | 63.630 | 1.00 39.15 | AAAA |
| ATOM | 364 | С | GLU A | | 45.301 | 42.737 | 63.681 | 1.00 39.29 | AAAA |
| ATOM | 365 | 0 | GLU A | | | 44.115 | 62.497 | 1.00 37.62 | AAAA |
| MOTA | 366 | N | LEU A | | 46.619 | | 61.211 | 1.00 35.88 | AAAA |
| MOTA | 367 | CA | LEU A | | 46.219 | 43.589 | 60.229 | 1.00 36.09 | AAAA |
| MOTA | 368 | CB | LEU A | | 46.125 | 44.750 | | 1.00 36.50 | AAAA |
| ATOM | 369 | CG | LEU A | | 45.608 | 44.550 | .58.817 | 1.00 36.66 | AAAA |
| ATOM | 370 | CD1 | LEU A | 46 | 44.182 | 44.021 | 58.843 | 1.00 35.85 | AAAA |
| ATOM | 371 | CD2 | LEU A | 46 | 45.646 | 45.893 | 58.113 | 1.00 34.97 | AAAA |
| ATOM | 372 | С | LEU A | 46 | 47.211 | 42.542 | 60.714 | | AAAA |
| ATOM | 373 | Ō | LEU A | | 48.424 | 42.670 | 60.900 | 1.00 35.72 | AAAA |
| ATOM | 374 | N | ILE A | A 47 | 46.680 | 41.484 | 60.118 | 1.00 33.25 | |
| | 375 | CA | ILE | | 47.497 | 40.411 | 59.560 | 1.00 30.92 | AAAA |
| ATOM | 376 | CB | ILE | _ | 47.144 | 39.024 | 60.167 | 1.00 31.22 | AAAA |
| ATOM | 377 | | ILE | | 48.093 | 37.97¢ | | | AAAA |
| ATOM | | | ILE | | 47.220 | 39.063 | 61.694 | 1.00 32.04 | AAAA |
| ATOM | 378 | | ILE | | 48.596 | 39.241 | 62.242 | 1.00 34.13 | AAAA |
| ATOM | 379 | | | | 47.138 | 40.381 | | 1.00 29.70 | AAAA |
| ATOM | 380 | C | ILE . | | 45.956 | 40.373 | | | AAAA |
| MOTA | 381 | 0 | ILE . | | 48.150 | 40.380 | | | AAAA |
| ATOM | 382 | N | LYS . | | | 40.349 | | | AAAA |
| ATOM | 383 | CA | LYS . | | 47.920 | 40.727 | | | AAAA |
| ATOM | 384 | CB | LYS . | | 49.203 | | | | AAAA |
| MOTA | 385 | CG | LYS | | 49.116 | 40.695 | | | AAAA |
| MOTA | 386 | CD | LYS | A 48 | 50.464 | 41.104 | | | AAAA |
| ATOM | 387 | CE | LYS | | 50.493 | 40.893 | | | AAAA |
| ATOM | 388 | NZ | LYS | | 49.409 | 41.645 | | 1.00 29.68 | AAAA |
| | 389 | c | LYS | | 47.449 | | | | |
| ATOM | | o | LYS | | 48.024 | 37.938 | | | AAAA |
| ATOM | 390 | | SER | _ | 46.385 | 38.892 | | | AAAA |
| ATOM | 391 | N | SER | | 45.854 | | | 1.00 26.41 | AAAA |
| ATOM | 392 | CA | | | 44.514 | | 53.420 | 1.00 25.40 | AAAA |
| ATOM | 393 | CB | SER | | 43.541 | | | 1.00 25.58 | AAAA |
| ATOM | 394 | OG | | A . 49 | 46.814 | | | 1.00 26.03 | AAAA |
| MOTA | 395 | C | SER | | | | | | AAAA |
| ATOM | 396 | 0 | SER | A 49 | 47.462 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | - | | • |
| • | | | | | | | | | |

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| | | | | | 1.8 | | | | |
|--------------|------------|----------|----------------|------------|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 397 | N | ARG A | 50 | 46.910 | 35.576 | 53.354 | 1.00 25.51 | AAAA |
| MOTA | 398 | | ARG A | 50 | 47.755 | 34.794 | 52.474 | 1.00 25.45 | AAAA |
| ATOM | 399 | CB | ARG A | 50 | 48.807 | 33.985 | 53.252 | 1.00 25.85 | AAAA |
| ATOM | 400 | CG | ARG A | 50 | 48.229 | 32.819 | 54.009 | 1.00 27.16 | AAAA AAAA |
| ATOM | 401 | CD | ARG A | 50 | 49.280 | 31.995 | 54.720 | 1.00 27.57 | AAAA |
| ATOM | 402 | NE | ARG A | 50 | 48.673 | 30.896 | 55.482 | 1.00 27.90 1.00 28.34 | AAAA |
| MOTA | 403 | CZ | ARG A | 50 | 48.106 | 29.820 | 54.946 53.630 | 1.00 28.34 | AAAA |
| ATOM | 404 | | ARG A | 50 | 48.055 | 29.672 28.884 | 55.735 | 1.00 28.62 | AAAA |
| ATOM | 405 | | ARG A | 50 | 47.592 46.806 | 33.834 | 51.762 | 1.00 24.91 | AAAA |
| MOTA | 406 | C | ARG A | 50 50 | 45.740 | 33.510 | 52.283 | 1.00 23.57 | AAAA |
| ATOM | 407 | 0 | ARG A PRO A | 51 | 47.172 | 33.392 | 50.549 | 1.00 24.28 | AAAA |
| ATOM | 408 409 | И CD | PRO A | 51 | 48.361 | 33.761 | 49.770 | 1.00 24.13 | AAAA |
| ATOM ATOM | 410 | CA | PRO A | 51 | 46.355 | 32.462 | 49.776 | 1.00 24.18 | AAAA |
| ATOM | 411 | CB | PRO A | 51 | 47.012 | 32.512 | 48.390 | 1.00 24.24 | AAAA |
| ATOM | 412 | CG | PRO A | 51 | 47.766 | 33.862 | 48.405 | 1.00 24.11 | AAAA |
| ATOM | 413 | С | PRO A | 51 | 46.473 | 31.070 | 50.393 | 1.00 23.69 | AAAA AAAA |
| ATOM | 414 | 0 | PRO A | 51 | 47.545 | 30.680 | 50.839 50.422 | 1.00 24.13 1.00 23.36 | AAAA |
| ATOM | 415 | N | ALA A | 52 | 45.381 | 30.325 28.972 | 50.952 | 1.00 23.64 | AAAA |
| MOTA | 416 | CA | ALA A | 52 | 45.419 44.012 | 28.405 | 51.029 | 1.00 23.86 | AAAA |
| ATOM | 417 | CB | ALA A | 52 52 | 46.260 | 28.145 | 49.994 | 1.00 23.58 | AAAA |
| ATOM | 418 419 | С 0 | ALA A | 52 | 46.240 | 28.383 | 48.806 | 1.00 24.52 | AAAA |
| ATOM | 419 | N | THR A | 53 | 47.009 | 27.185 | 50.501 | 1.00 24.41 | AAAA |
| ATOM ATOM | 421 | CA | THR A | 53 | 47.815 | 26.352 | 49.628 | 1.00 26.26 | AAAA |
| ATOM | 422 | CB | THR A | 5 3 | 48.933 | 25.642 | 50.405 | 1.00 26.37 | AAAA |
| ATOM | 423 | OG1 | THR A | 53 | 48.355 | 24.763 | 51.375 | 1.00 26.51 | AAAA AAAA |
| ATOM | 424 | CG2 | THR A | 53 | 49.810 | 26.648 | 51.106 | 1.00 24.48 1.00 27.63 | AAAA |
| MOTA | 425 | C | THR A | 53 | 46.889 | 25.299 | 49.034 49.620 | 1.00 27.03 | AAAA |
| ATOM | 426 | 0 | THR A | 53 | 45.870 47.240 | 24.982 24.776 | 47.867 | 1.00 29.31 | AAAA |
| MOTA | 427 | N | LYS A | 54 54 | 46.450 | 23.752 | 47.189 | 1.00 30.61 | AAAA |
| ATOM | 428 | CA CB | LYS A | 54 | 47.249 | 23.182 | 46.015 | 1.00 31.68 | AAAA |
| ATOM | 429 430 | CG | LYS A | 54 | | 22.020 | 45.304 | 1.00 34.38 | AAAA |
| ATOM ATOM | 431 | CD | LYS A | 54 | 45.449 | 22.464 | 44.417 | 1.00 36.00 | AAAA |
| ATOM | 432 | CE | LYS A | 54 | 45.943 | 22.850 | 43.025 | 1.00 37.55 | AAAA |
| ATOM | 433 | NZ | LYS A | 54 | 46.425 | 21.664 | 42.236 | 1.00 37.57 | AAAA AAAA |
| ATOM | 434 | С | LYS A | 54 | 46.127 | 22.640 | 48.170 | 1.00 31.26 1.00 31.72 | AAAA |
| ATOM | 435 | 0 | LYS A | 54 | 45.025 | 22.097 | 48.176 49.006 | 1.00 31.72 | AAAA |
| MOTA | 436 | N | GLU A | 55 | 47.102 46.961 | 22.312 21.260 | 50.011 | 1.00 32.29 | AAAA |
| ATOM | 437 | CA | GLU A | 55 55 | 48.266 | 21.089 | 50.778 | 1.00 34.43 | AAAA |
| ATOM | 438 439 | CB CG | GLU A | 55 | 48.265 | 19.901 | 51.706 | 1.00 38.39 | AAAA |
| MOTA | 440 | CD | GLU A | 55 | 49.513 | 19.839 | 52.584 | 1.00 41.46 | AAAA |
| MOTA MOTA | 441 | | GLU A | 55 | 49.745 | 18.770 | 53.200 | 1.00 43.30 | AAAA |
| MOTA | 442 | | GLU A | 55 | 50.245 | 20.859 | 52.672 | 1.00 42.45 | AAAA AAAA |
| ATOM | 443 | C | GLU A | 5 5 | 45.851 | 21.555 | 51.013 | 1.00 30.43 1.00 30.59 | AAAA |
| MOTA | 444 | 0 | GLU A | 55 | 45.048 | 20.681 | 51.332 51.517 | 1.00 30.33 | AAAA |
| MOTA | 445 | N | GLU A | 56 | 45.822 | 22.782 23.164 | 52.488 | 1.00 27.69 | AAAA |
| ATOM | 446 | CA | GLU A | 56 | 44.812 45.078 | 24.588 | 52.989 | 1.00 27.90 | AAAA |
| ATOM | 147 | CB | GLU A | 56 56 | 46.434 | 24.721 | 53.670 | 1.00 26.64 | AAAA |
| ATOM | 448 449 | CG CD | GLU A GLU A | 56 | 46.769 | 26.135 | 54.098 | 1.00 26.35 | AAAA |
| MOTA | 449 | | GLU A | 56 | 46.615 | 27.057 | 53.265 | 1.00 25.12 | AAAA |
| ATOM ATOM | 451 | | GLU A | 56 | 47.213 | 26.315 | 55.255 | 1.00 25.70 | AAAA |
| ATOM | 452 | C | GLU A | 56 | 43.408 | 23.043 | 51.914 | 1.00 26.99 | AAAA |
| ATOM | 453 | 0 | GLU A | 56 | 42.495 | 22.574 | 52.588 | 1.00 26.25 | AAAA AAAA |
| MOTA | 454 | N | LEU A | 57 | 43.252 | 23.447 | 50.659 | 1.00 27.26 1.00 27.17 | AAAA |
| ATOM | 455 | CA | LEU A | 57 | 41.965 | 23.389 | 49.967 | 1.00 27.17 | AAAA |
| ATOM | 456 | CB | LEU A | 57 | 42.077 | 24.063 25.545 | 48.596 48.656 | 1.00 27.64 | AAAA |
| ATOM | 457 | CG | LEU A | 57 | 42.491 | 25.545 | 47.269 | 1.00 26.66 | AAAA |
| ATOM | 458 | | LEU A | 57 57 | 42.770 41.389 | | | 1.00 26.92 | AAAA |
| ATOM | 159 | | LEU A | 57 57 | 41.552 | 21.946 | | 1.00 27.26 | AAAA |
| ATOM | 460 461 | 0 | LEU A | 57 | 40.363 | 21.612 | | 1.00 27.53 | AAAA |
| ATOM | 461 462 | N | LEU A | 58 | 42.547 | 21.085 | | 1.00 27.42 | AAAA |
| ATOM | 302 | 41 | -20 A | | | | • | | • |

| imose | 463 | CA LEU A | 58 | 42.293 | 19.675 | 49.457 | 1.00 26.10 | AAAA |
|--------|------------|-----------|----|---------------------------|--------|----------|------------|------|
| ATOM | 463 464 | | 58 | 43.486 | 19.019 | 48.794 | 1.00 25.43 | AAAA |
| ATOM | 465 | | 58 | 43.623 | 19.577 | 47.385 | 1.00 26.66 | AAAA |
| MOTA | 465 | | 58 | 44.760 | 18.884 | 46.705 | 1.00 27.12 | AAAA |
| ATOM | | | 58 | 42.334 | 19.355 | 46.600 | 1.00 26.43 | AAAA |
| MOTA | 467 | | 58 | 41.938 | 18.956 | 50.731 | 1.00 25.79 | AAAA |
| ATOM | 468 | | 58 | 41.648 | 17.763 | 50.692 | 1.00 26.50 | AAAA |
| ATOM | 469 | • | 59 | 41.977 | 19.666 | 51.858 | 1.00 24.91 | AAAA |
| MOTA | 470 | | 59 | 41.595 | 19.070 | 53.136 | 1.00 25.15 | AAAA |
| MOTA | 471 | CA LEU A | 59 | 41.958 | 19.991 | 54.322 | 1.00 25.44 | AAAA |
| ATOM | 472 | CB LEU A | 59 | 43.423 | 20.280 | 54.710 | 1.00 24.67 | AAAA |
| MOTA | 473 | CG LEU A | 59 | 43.502 | 21.461 | 55.652 | 1.00 23.70 | AAAA |
| MOTA | 474 | | 59 | 44.044 | 19.044 | 55.357 | 1.00 24.08 | AAAA |
| MOTA | 475 | CD2 LEU A | 59 | 40.074 | 18.870 | 53.090 | 1.00 25.41 | AAAA |
| ATOM | 476 | C LEU A | 59 | 39.503 | 18.266 | 53.993 | 1.00 25.88 | AAAA |
| ATOM | 477 | O LEU A | 60 | 39.436 | 19.392 | 52.031 | 1.00 25.05 | AAAA |
| ATOM | 478 | N PHE A | 60 | 37.983 | 19.276 | 51.823 | 1.00 24.11 | AAAA |
| MOTA | 479 | CA PHE A | 60 | 37.250 | 20.476 | 52.440 | 1.00 21.80 | AAAA |
| MOTA | 480 | CB PHE A | | 35.778 | 20.534 | 52.098 | 1.00 20.07 | AAAA |
| MOTA | 481 | CG PHE A | 60 | 34.917 | 19.501 | 52.462 | 1.00 19.27 | AAAA |
| MOTA | 482 | CD1 PHE A | 60 | 35.249 | 21.628 | 51.399 | 1.00 19.82 | AAAA |
| MOTA | 483 | CD2 PHE A | 60 | 33.550 | 19.557 | 52.136 | 1.00 19.26 | AAAA |
| MOTA | 484 | CE1 PHE A | 60 | 33.890 | 21.688 | 51.071 | 1.30 17.45 | AAAA |
| MOTA | 485 | CE2 PHE A | 60 | 33.042 | 20.652 | 51.440 | 1.00 17.92 | AAAA |
| ATOM | 486 | CZ PHE A | 60 | 37.557 | 19.139 | 50.345 | 1.00 24.02 | AAAA |
| MOTA | 487 | C PHE A | 60 | 36.846 | 18.201 | 49.974 | 1.00 23.27 | AAAA |
| ATOM | 488 | O PHE A | 60 | 37.982 | 20.079 | 49.511 | 1.00 24.40 | AAAA |
| MOTA | 489 | N HIS A | 61 | 37.526 | 20.073 | 48.099 | 1.00 25.04 | AAAA |
| ATOM | 490 | CA HIS A | 61 | 37.768 | 21.449 | 47.494 | 1.00 24.19 | AAAA |
| . ATOM | 491 | CB HIS A | 61 | 36.744 | 22.429 | 47.979 | 1.00 24.44 | AAAA |
| ATOM | 492 | CG HIS A | 61 | | 22.559 | 47.683 | 1.00 24.12 | AAAA |
| ATOM | 493 | CD2 HIS A | 61 | 35.429 37.038 | 23.444 | 48.864 | 1.00 24.36 | AAAA |
| ATOM | 494 | ND1 HIS A | 61 | 35.952 | 24.159 | | 1.00 23.18 | AAAA |
| ATOM | 495 | CE1 HIS A | 61 | | 23.643 | 48.385 | 1.00 23.91 | AAAA |
| MOTA | 496 | NE2 HIS A | 61 | 34.962 | 19.054 | 47.253 | 1.00 25.60 | AAAA |
| MOTA | 497 | C HIS A | 61 | 38.416 | 18.805 | 47.498 | 1.00 26.94 | AAAA |
| MOTA | 498 | O HIS A | 61 | 39.596 3 7 .754 | 18.496 | 46.244 | 1.00 26.68 | AAAA |
| ATOM | 499 | N THR A | 62 | | 17.522 | 45.333 | 1.00 28.17 | AAAA |
| MOTA | 500 | CA THR A | 62 | 38.369 37.290 | 16.695 | 44.614 | 1.00 28.15 | AAAA |
| ATOM | 501 | CB THR A | 62 | 36.544 | 17.541 | 43.731 | 1.00 28.10 | AAAA |
| MOTA | 502 | OG1 THR A | 62 | 36.334 | 16.094 | 45.629 | 1.00 28.24 | AAAA |
| MOTA | 503 | CG2 THR A | 62 | 39.226 | 18.217 | 44.278 | 1.00 29.28 | AAAA |
| MOTA | 504 | C THR A | 62 | 38.876 | 19.286 | 43.792 | 1.00 29.52 | AAAA |
| ATOM | 505 | O THR A | 62 | 40.344 | 17.606 | 43.912 | 1.00 31.33 | AAAA |
| MOTA | 506 | N GLU A | 63 | 41.249 | 18.202 | 42.928 | 1.00 32.42 | AAAA |
| MOTA | 507 | CA GLU A | 63 | 42.333 | 17.219 | 42.536 | 1 00 34.37 | AAAA |
| MOTA | 508 | CB GLU A | 63 | 43.304 | 16.869 | 43.609 | 1 00 37.20 | AAAA |
| MOTA | 509 | CG GLU A | 63 | 44.427 | 16.022 | 43.052 | 1 00 38.79 | AAAA |
| MOTA | 510 | CD GLU A | 63 | 45.100 | 16.499 | | 1.00 37.96 | AAAA |
| MOTA | 511 | OE1 GLU A | 63 | 44.619 | 14.892 | 43.564 | 1.00 39.68 | AAAA |
| MOTA | 512 | OE2 GLU A | 63 | 40.607 | 18.687 | 41.639 | | AAAA |
| MOTA | 513 | C GLU A | 63 | 40.824 | 19.816 | | 1.00 32.10 | AAAA |
| ATOM | 514 | O GLU A | 63 | 39.845 | 17.814 | | 1.00 31.52 | AAAA |
| ATOM | 515 | N ASP A | 64 | 39.204 | 18.165 | | 1.00 31.36 | AAAA |
| MOTA | 516 | CA ASP A | 64 | 38.301 | 17.018 | | | AAAA |
| MOTA | 517 | CB ASP A | 64 | 30.301 | 16.694 | | 1.00 37.38 | AAAA |
| ATOM | 518 | CG ASP A | 64 | | 15.801 | | | AAAA |
| ATOM | 519 | OD1 ASP A | 64 | 36.375 | 17.332 | | | AAAA |
| ATOM | 520 | OD2 ASP A | 64 | 37.188 | 19.465 | | | AAAA |
| MOTA | 521 | C ASP A | 64 | 38.412 | | | | AAAA |
| ATOM | 522 | A PZA C | 64 | 38.462 | 20.331 | | | AAAA |
| ATOM | 523 | N TYR A | 65 | 37.695 | 19.608 | | | AAAA |
| ATCM | 524 | | 65 | 36.918 | 20.814 | | | AAAA |
| ATOM | 525 | CB TYR A | 65 | 36.010 | | | | AAAA |
| ATOM | 526 | | 65 | 35.339 | | | | AAAA |
| ATOM | 527 | CD1 TYR A | 65 | 34.525 | 22.636 | | | AAAA |
| ATOM | 528 | | 65 | 33.914 | 23.823 | , 42.300 | 1.00 -0.01 | |
| | | | | | | | | |

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| | | | | | _ | | | | |
|------|-----|------|-------|-----------|--------|----------|--------|------------|--------|
| | | | | c = | 35.525 | 22.486 | 44.136 | 1.00 24.65 | AAAA |
| MOTA | | _ | ryr A | 65 | 34.920 | 23.677 | 44.497 | 1.00 25.86 | AAAA |
| ATOM | 530 | _ | ryr A | 65 | | | 43.576 | 1.00 26.69 | AAAA |
| MOTA | 531 | CZ 7 | ryr a | 65 | 34.110 | 24.349 | | 1.00 27.20 | AAAA |
| MOTA | 532 | OH : | ryr A | 65 | 33,499 | 25.543 | 43.924 | | |
| | | | TYR A | 65 | 37.814 | 22.022 | 41.464 | 1.00 24.91 | AAAA |
| ATOM | | | TYR A | 65 | 37.460 | 23.129 | 41.096 | 1.00 25.62 | AAAA |
| MOTA | | | | | 38.965 | 21.812 | 42.080 | 1.00 23.20 | AAAA |
| ATOM | | - | ILE A | 56 | | 22.902 | 42.328 | 1.00 22.33 | AAAA |
| ATOM | 536 | CA : | ILE A | 56 | 39.877 | | 43.402 | 1.00 21.45 | AAAA |
| MOTA | 537 | CB : | ILE A | 66 | 40.924 | 22.520 | | | AAAA |
| ATOM | | CG2 | ILE A | 56 | 41.927 | 23.652 | 43.617 | 1.00 20.00 | AAAA |
| | | | ILE A | 66 | 40.220 | 22.289 | 44.729 | 1.00 20.16 | |
| MOTA | | | ILE A | 56 | 39.528 | 23.523 | 45.228 | 1.00 19.68 | , AAAA |
| MOTA | | | | | 40.558 | 23.261 | 41.023 | 1.00 22.68 | AAAA |
| MOTA | | | ILE A | 66 | 40.636 | 24.425 | 40.665 | 1.00 23.19 | AAAA |
| MOTA | 542 | | ILE A | 66 | | 22.262 | 40.295 | 1.00 22.96 | AAAA |
| ATOM | 543 | N . | ASN A | 67 | 41.036 | | 39.029 | 1.00 23.92 | AAAA |
| ATOM | 544 | CA . | ASN A | 67 | 41.698 | 22.545 | | 1.00 24.24 | AAAA |
| ATOM | 545 | CB . | ASN A | 67 | 42.292 | 21.261 | 38.395 | | AAAA |
| | 546 | | ASN A | 67 | 43.344 | 20.588 | 39.289 | 1.00 23.38 | |
| MOTA | | | ASN A | 67 | 44.196 | 21.256 | 39.859 | 1.00 23.47 | AAAA |
| MOTA | 547 | | | 67 | 43.290 | 19.258 | 39.392 | 1.00 23.20 | AAAA |
| ATOM | 548 | | ASN A | | 40.717 | 23.216 | 38.063 | 1.00 23.82 | AAAA |
| ATOM | 549 | _ | ASN A | 67 | | 23.996 | 37.204 | 1.00 24.63 | AAAA |
| ATOM | 550 | 0 | ASN A | 67 | 41.123 | | 38.213 | 1.00 24.08 | AAAA |
| ATOM | 551 | N | THR A | 68 | 39.427 | 22.928 | | 1.00 25.28 | AAAA |
| MOTA | 552 | CA | THR A | 68 | 38.428 | 23.534 | 37.343 | | AAAA |
| | 553 | | THR A | 58 | 37.030 | 22.904 | 37.525 | 1.00 24.55 | |
| ATOM | | | THR A | 68 | 37.090 | 21.500 | 37.258 | 1.00 24.64 | AAAA |
| MOTA | 554 | | | 58 | 36.049 | 23.534 | 36.564 | 1.00 23.58 | AAAA |
| MOTA | 555 | | THR A | | 38.322 | 25.023 | 37.664 | 1.00 26.31 | AAAA |
| MOTA | 556 | С | THR A | 68 | | 25.854 | 36.771 | 1.00 26.69 | AAAA |
| ATOM | 557 | 0 | THR A | 68 | 38.114 | | 38.945 | 1.00 26.59 | KAAA |
| MOTA | 558 | N | LEU A | 69 | 38.462 | 25.351 | | 1.00 27.05 | AAAA |
| ATOM | 559 | CA | LEU A | 59 | 38.381 | 26.729 | 39.378 | | AAAA |
| MOTA | 560 | | LEU A | | 38.321 | 26.807 | 40.904 | 1.00 27.15 | |
| | 561 | | LEU A | | 37.003 | 26.397 | 41.551 | 1.00 25.68 | AAAA |
| ATOM | | | LEU A | 69 | 37.088 | 26.491 | 43.062 | 1.00 26.30 | AAAA |
| MOTA | 562 | | | | 35.933 | 27.316 | 41.044 | 1.00 26.14 | AAAA |
| ATOM | 563 | | LEU A | | 39.570 | 27.508 | 38.867 | 1.00 28.44 | AAAA |
| ATOM | 564 | С | LEU A | | | 28.619 | 38.356 | 1.00 28.59 | AAAA |
| MOTA | 565 | 0 | LEU Y | | 39.425 | | 39.009 | 1.00 29.31 | AAAA |
| MOTA | 566 | N | MET A | . 70 | 40.748 | 26.914 | | 1.00 29.89 | AAAA |
| ATOM | 567 | CA | MET A | . 70 | 41.981 | 27.536 | 38.571 | 1.00 31.04 | AAAA |
| MOTA | 568 | CB | MET A | 70 | 43.160 | 26.692 | 39.044 | 1.00 31.04 | AAAA |
| | 569 | ĊĠ | MET A | | 43.164 | 26.528 | 40.562 | 1.00 31.79 | |
| ATOM | | SD | MET A | | 44.608 | 25.684 | 41.183 | 1.00 32.58 | AAAA |
| MOTA | 570 | | | | 45.859 | 26.820 | 40.670 | 1.00 30.82 | AAAA |
| ATOM | 571 | CE | MET A | | 42.017 | 27.723 | 37.057 | 1.00 30.36 | AAAA |
| MOTA | 572 | С | MET ? | | | 28.769 | 36.559 | 1.00 30.18 | AAAA |
| MOTA | 573 | 0 | MET 2 | | 42.462 | | 36.328 | 1.00 30.34 | AAAA |
| MOTA | 574 | - N | GLU 3 | 71 | 41.538 | 26.719 | | 1.00 30.73 | AAAA |
| ATOM | 575 | CA | GLU A | 71 | 41.519 | 26.795 | 34.874 | | AAAA |
| | 576 | CB | GLU A | | 41.140 | 25.442 | 34.266 | 1.00 33.47 | |
| ATOM | 577 | CG | GLU A | | 41.122 | 25.430 | 32.731 | 1.00 37.11 | AAAA |
| ATOM | | | | | 42.513 | 25.676 | 32.093 | 1.00 40.49 | AAAA |
| ATOM | 578 | CD | GLU A | | 42.570 | 25.798 | 30.844 | 1.00 41.95 | AAAA |
| MOTA | 579 | | GLU A | | | 25.738 | | | AAAA |
| ATOM | 580 | OE2 | GLU ? | | 43.541 | | | | AAAA |
| ATOM | 581 | С | GLU A | | 40.537 | 27.851 | | | AAAA |
| MOTA | 582 | 0 | GLU 2 | 71 | 40.852 | 28.642 | | | AAAA |
| | 583 | N | ALA A | | 39.352 | 27.855 | | | |
| MOTA | 584 | CA | ALA A | - | 38.296 | 28.790 | 34.635 | 1.00 29.88 | AAAA |
| MOTA | | | | - | 37.022 | 28.432 | 35.374 | 1.00 29.07 | AAAA |
| MOTA | 585 | СВ | ALA : | | 38.667 | | | 1.00 30.78 | АААА |
| ATOM | 586 | C | ALA A | | | | | | AAAA |
| MOTA | 587 | O | ALA A | | 38.359 | | | | AAAA |
| ATOM | 588 | N | GLU : | A 73 | 39.336 | | | | AAAA |
| ATOM | 589 | CA | GLU : | | 39.710 | | | | AAAA |
| | 590 | CB | GLU | | 40.243 | | | | |
| ATOM | | | GLU | | 40.643 | | 38.198 | | AAAA |
| ATOM | 591 | CG | | | 41.076 | | | 1.00 28.77 | AAAA |
| ATOM | 592 | CD | GLU . | | 40.239 | | | 1.00 28.94 | AAAA |
| ATOM | 593 | OEI | GLU . | A 73 | | | | | AAAA |
| ATOM | 594 | OE2 | GLU | A 73 | 42.258 | . 33.133 | , | | • |
| | | | | | | • | | | |

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| • | | | | | 1. | iguie 17 | | | | | |
|--------------|------------|---------|------------|------|----|------------------|------------------|------------------|--------------------------|------------|--------------|
| | 505 | _ | GLU A | . 73 | | 40.726 | 32.461 | 35.378 | 1.00 33.54 | AA | |
| ATOM | 595 506 | - | GLU A | | | 40.456 | 33.499 | 34.767 | 1.00 34.93 | AA | |
| ATOM | 596 | Ŋ | ARG A | | | 41.885 | 31.832 | 35.214 | 1.00 34.35 | AA. | |
| MOTA | 597 598 | CA | ARG A | - | | 42.890 | 32.428 | 34.334 | 1.00 36.04 | | AA |
| ATOM | 599 | CB | ARG A | | | 44.238 | 31.710 | 34.482 | 1.00 36.92 | AA | |
| ATOM | 600 | CG | ARG A | | | 44.327 | 30.313 | 33.923 | 1.00 38.14 | | AA |
| ATOM- | 601 | CD | ARG A | | | 45.508 | 29.589 | 34.543 | 1.00 39.55 | | AA. |
| MOTA | 602 | NE | ARG A | - | | 45.893 | 28.404 | 33.785 | 1.00 42.02 | | AA |
| ATOM | 603 | CZ | ARG A | - | | 46.632 | 28.436 | 32, 675 | 1.00 42.69 | | AA · |
| MOTA | 604 | | ARG A | | | 47.071 | 29.593 | 32.191 | 1.00 42.76 | | AA |
| MOTA MOTA | 605 | | ARG A | | | 46.933 | 27.309 | 32.046 | 1.00 42.92 | | AA |
| ATOM | 606 | C | ARG A | | | 42.476 | 32.532 | 32.864 | 1.00 36.56 | | AA |
| ATOM | 607 | Ö | ARG A | | - | 42.842 | 33.493 | 32.187 | 1.00 37.73 | | AA |
| ATOM | 608 | N | SER A | | | 41.711 | 31.567 | 32.367 | 1.00 36.60 | | AAA |
| ATOM | 609 | CA | SER A | | | 41.248 | 31.622 | 30.987 | 1.00 36.82 | AA - AA | AAA |
| ATOM | 610 | CB | SER A | A 75 | | 40.916 | 30.218 | 30.478 | 1.00 36.10 1.00 36.39 | | AA. |
| ATOM | 611 | OG | SER A | | | 39.736 | 29.723 | 31.083 | 1.00 36.39 | | LAA |
| ATOM | 612 | С | SER A | | | 39.980 | 32.476 | 31.001 | 1.00 36.25 | | AAA |
| ATOM | 613 | . 0 | SER A | | | 39.401 | 32.791 | 29.963 | 1.00 37.62 | | AA. |
| ATOM | 614 | N | GLN A | | | 39.568 | 32.845 | 32.208 32.427 | 1.00 37.02 | | AAA |
| ATOM | 615 | CA | GLN A | | | 38.368 | 33.639 | 32.049 | 1.00 37.32 | | AAA |
| ATOM | 616 | CB | GLN A | | | 38.613 | 35.100 | 32.717 | 1.00 40.67 | | AAA |
| MOTA | 617 | CG | GLN A | | | 37.630 | 36.048 36.298 | 34.199 | 1.00 41.40 | | AAA |
| ATOM | 618 | CD | GLN A | | | 37.929 | 35.379 | 34.973 | 1.00 40.79 | | AAA |
| MOTA | 619 | | GLN A | | | 38.226 37.833 | 37.556 | 34.597 | 1.00 42.32 | | AAA |
| MOTA | 620 | NE2 | | | | 37.223 | 33.064 | 31.600 | 1.00 37.75 | | AAA |
| ATOM | 621 | C | GLN A | | | 36.521 | 33.789 | 30.901 | 1.00 38.13 | | AAA |
| ATOM | 622 | 0 | GLN . | | • | 37.045 | 31.749 | 31.685 | 1.00 37.52 | A | AAA |
| MOTA | 623 | N | SER | | | 35.990 | 31.061 | 30.950 | 1.00 37.75 | A. | AAA |
| ATOM | 624 | CA | SER . | | | 36.537 | 30.440 | 29.664 | 1.00 37.90 | | AAA |
| MOTA | 625 | CB | SER . | | | 36.851 | 31.441 | 28.724 | 1.00 40.32 | | AAA |
| MOTA | 626 627 | C OĠ | SER | | | 35.338 | 29.960 | 31.757 | 1.00 37.55 | | AAA |
| ATOM | 628 | 0 | SER | | | 35.790 | 29.620 | 32.846 | 1.00 36.81 | | AAA |
| MOTA | 629 | N. | VAL | | | 34.264 | 29.412 | 31.198 | | | AAA |
| ATOM ATOM | 630 | CA | VAL | | | 33.538 | 28.309 | 31.812 | 1.00 37.99 | | AAA |
| ATOM | 631 | CB | VAL | | | 32.027 | 28.514 | 31.715 | 1.00 37.19 | | AAA |
| ATOM | 632 | | VAL | A 78 | | 31.310 | 27.439 | 32.497 | 1.00 36.84 | | AAA AAA |
| ATOM | 633 | | VAL | | | 31.662 | 29.906 | 32.201 | 1.00 37.60 1.00 38.28 | | AAA |
| MOTA | 634 | С | VAL | A 78 | | 33.918 | 27.089 | 30.976 | 1.00 38.28 | | AAA |
| ATOM | 635 | 0 | VAL | | | 33.497 | 26.959 | 29.819 | 1.00 37.69 | | AAA |
| ATOM | 636 | N | PRO | | | 34.734 | 26.187 | 31.537 32.869 | 1.00 37.65 | | AAA |
| ATOM | 637 | CD | PRO | | | 35.347 | 26.167 | 30.797 | 1.00 37.53 | | AAA |
| ATOM | 638 | CA | PRO | | | 35.146 | 24.998 24.325 | 31.759 | 1.00 37.45 | | AAA |
| ATOM | 639 | CB | PRO | | | 36.127 | 25.489 | 32.557 | 1.00 37.65 | · A | AAA |
| ATOM | 640 | CG | PRO | | | 36.655 33.980 | 24.089 | 30.434 | 1.00 37.20 | | AAA |
| ATOM | 641 | , C | PRO | | | 32.958 | 24.050 | 31.120 | 1.00 36.43 | Α | AAA |
| MOTA | 642 | 0 | PRO | | | 34.154 | 23.363 | 29.338 | 1.00 37.42 | A | AAA |
| ATOM | 643 | N | LYS | | | 33.160 | 22.423 | 28.855 | 1.00 37.35 | A | AAA |
| ATOM | 644 | CA | LYS | | | 33.757 | 21.586 | 27.725 | 1.00 37.99 | | AAA |
| ATOM | 645 | CB | LYS LYS | | | 32.928 | 20.379 | 27.280 | 1.00 38.94 | | AAA |
| ATOM | 646 647 | CD | LYS | | | 31.835 | 20.710 | | 1.00 39.07 | | AAA |
| ATOM | .648 | CE | LYS | | | 31.320 | 19.402 | | 1.00 40.43 | | AAAA |
| ATOM | 649 | NZ | LYS | | | 30.498 | 19.543 | 24.450 | 1.00 40.48 | | AAA |
| ATOM | 650 | C | LYS | | | 32.752 | 21.515 | | 1.00 36.85 | | AAA |
| ATOM | 651 | ō | LYS | | | 33.610 | 20.942 | | | | AAA |
| ATOM | 652 | | GLY | | | 31.443 | | | | | AAAA |
| MOTA | 653 | CA | GLY | | | 30.903 | 20.570 | | | _ | AAAA |
| atom atom | -654 | C | GLY | | | 31.110 | 21.054 | | | | AAAA |
| ATOM | 655 | | GLY | | | 30.749 | | 33.644 | | | AAAA AAAA |
| ATOM | 656 | | ALA | | | 31.677 | | | 1.00 35.17 | | AAAA |
| ATOM | 657 | | ALA | | | 31.919 | | 34.213 | | | aaaa Aaaa |
| ATOM | 658 | | ALA | | 2 | 33.076 | | | | | AAAA |
| ATOM | 659 | | ALA | | | 30.674 | | | | | AAAA |
| ATOM | 660 | | ALA | A 8 | 2 | 30.451 | . 23.332 | 36.001 | . 1.00 33.02 | • | • |
| | | | | | | | | | | | |

| | 661 | N | ARG A | 83 | 29.858 | 23.960 | 33.932 | 1.00 34.77 | AAAA |
|--------|-----------------|-----|-------|----|---------|----------|--------|------------|------|
| MOTA | 661 | | ARG A | 83 | 28.637 | 24.613 | 34.361 | 1.00 35.34 | AAAA |
| MOTA | 662 | CA | | | | 25.180 | 33.150 | 1.00 36.26 | AAAA |
| ATOM | 663 | CB | ARG A | 83 | 27.899 | | 33.464 | 1.00 37.09 | AAAA |
| ATOM | 664 | CG | ARG A | 83 | 27.045 | 26.395 | | | AAAA |
| ATOM | 665 | CD | ARG A | 83 | 26.209 | 26.141 | 34.686 | 1.00 37.48 | |
| ATOM | 666 | NE | ARG A | 83 | 25.475 | 27.310 | 35.134 | 1.00 37.35 | AAAA |
| MOTA | 667 | CZ | ARG A | 83 | 24.711 | 27.311 | 36.218 | 1.00 37.77 | AAAA |
| | 668 | | ARG A | 83 | 24.606 | 26.204 | 36.940 | 1.00 37.29 | AAAA |
| ATOM | | | ARG A | 83 | 24.040 | 28.401 | 36.568 | 1.00 38.34 | AAAA |
| MOTA | 669 | | | | 27.739 | 23.603 | 35.065 | 1.00 36.30 | AAAA |
| MOTA | 670 | С | ARG A | 83 | | 23.854 | 36.154 | 1.00 36.17 | AAAA |
| ATOM | 671 | 0 | ARG A | 83 | 27.232 | | 34.431 | 1.00 37.19 | AAAA |
| ATOM | 672 | N | GLU A | 84 | 27.565 | 22.450 | | 1.00 37.13 | AAAA |
| ATOM | 673 | CA | GLU A | 84 | 26.721 | 21.382 | 34.948 | | |
| ATOM | 674 | CB | GLU A | 84 | 26.466 | 20.375 | 33.833 | 1.00 40.55 | AAAA |
| ATOM | 675 | CG | GLU A | 84 | 25.643 | . 19.171 | 34.232 | 1.00 43.12 | AAAA |
| ATOM | 676 | CD | GLU A | 84 | 25.362 | 18.268 | 33.046 | 1.00 44.98 | AAAA |
| | 677 | | GLU A | 84 | 24.573 | 17.301 | 33.195 | 1.00 46.36 | AAAA |
| ATOM | | | GLU A | 84 | 25.937 | 18.532 | 31.962 | 1.00 44.94 | AAAA |
| ATOM | 678 | | GLU A | 84 | 27,290 | 20.657 | 36.158 | 1.00 37.07 | AAAA |
| MOTA | 679 | С | | | 26.642 | 20.555 | 37.199 | 1.00 36.17 | AAAA |
| ATOM | 680 | 0 | GLU A | 84 | 28.506 | 20.152 | 35.999 | 1.00 36.23 | AAAA |
| MOTA | 681 | N | LYS A | 85 | _ | 19.412 | 37.043 | 1.00 35.36 | AAAA |
| MOTA | 682 | CA | LYS A | 85 | 29.202 | | | 1.00 36.96 | AAAA |
| ATOM | 683 | CB | LYS A | 85 | 30.449 | 18.761 | 36.437 | 1.00 30.90 | AAAA |
| ATOM | 584 | CG | LYS A | 85 | 31.394 | 18.158 | 37.465 | | |
| ATOM | 685 | CD | LYS A | 85 | 30.995 | 16.766 | 37.919 | 1.00 40.59 | AAAA |
| ATOM | 686 | CE | LYS A | 85 | 31.508 | 15.719 | 36.933 | 1.00 41.88 | AAAA |
| ATOM | 687 | NZ | LYS A | 85 | 32.998 | 15.817 | 36.757 | 1.00 42.00 | AAAA |
| | 688 | C | LYS A | 85 | 29.620 | 20.202 | 38.289 | 1.00 33.86 | AAAA |
| ATOM | 689 | Ö | LYS A | 85 | 29.576 | 19.679 | 39.404 | 1.00 33.82 | AAAA |
| ATOM | 690 | N | TYR A | 86 | 30.014 | 21.458 | 38.097 | 1.00 32.06 | AAAA |
| ATOM | | | TYR A | 86 | 30.514 | 22.279 | 39.194 | 1.00 29.44 | AAAA |
| MOTA | 691 | CA | | 86 | 31.956 | 22.683 | 38.875 | 1.00 29.97 | AAAA |
| MOTA | 692 | CB | TYR A | | 32.872 | 21.496 | 38.621 | 1.00 29.99 | AAAA |
| ATOM | 693 | CG | TYR A | 86 | 33.281 | 20:666 | 39.666 | 1.00 29.24 | AAAA |
| MOTA | 694 | | TYR A | 86 | | 19.582 | 39.437 | 1.00 29.85 | AAAA |
| ATOM | 695 | | TYR A | 86 | 34.126 | | 37.329 | 1.00 30.16 | AAAA |
| ATOM | 696 | CD2 | TYR A | 86 | .33.329 | 21.204 | 37.087 | 1.00 30.10 | AAAA |
| ATOM | 697 | CE2 | | 86 | 34.173 | 20.118 | | 1.00 29.79 | AAAA |
| ATOM | 698 | CZ | TYR A | 86 | 34.570 | 19.313 | 38.148 | 1.00 29.48 | AAAA |
| ATOM | 699 | OH | TYR A | 86 | 35.414 | 18.253 | 37.923 | | AAAA |
| ATOM | 700 | С | TYR A | 86 | 29.705 | 23.509 | 39.572 | 1.00 27.81 | AAAA |
| ATOM | 701 | 0 | TYR A | 86 | 30.052 | 24.202 | 40.524 | 1.00 27.56 | |
| ATOM | 702 | N | ASN A | 87 | 28.642 | 23.784 | 38.828 | 1.00 26.60 | AAAA |
| ATOM | 703 | CA | ASN A | 87 | 27.777 | 24.924 | 39.111 | 1.00 26.56 | AAAA |
| | 704 | CB | ASN A | 87 | 27.172 | 24.772 | 40.508 | 1.00 26.39 | AAAA |
| MOTA | 705 | CG | ASN A | 87 | 25.863 | 25.544 | 40.684 | 1.00 26.64 | AAAA |
| MOTA | 706 | | ASN A | 87 | 25.335 | 25.632 | 41.790 | 1.00 26.84 | AAAA |
| MOTA | 707 | | ASN A | 87 | 25.330 | 26.084 | 39.597 | 1.00 26.33 | AAAA |
| ATOM | | | ASN A | 87 | 28.587 | 26.217 | 39.024 | 1.00 26.40 | AAAA |
| ATOM | 708 | C | | | 28.430 | 27.129 | 39.832 | 1.00 24.80 | AAAA |
| MOTA | 709 | 0 | ASN A | | 29.448 | 26.273 | 38.015 | 1.00 27.57 | AAAA |
| MOTA | 710 | N | ILE A | 88 | | 27.409 | 37.767 | 1.00 27.88 | AAAA |
| ATOM | 711 | CA | ILE A | | 30.330 | | 37.648 | 1.00 27.38 | AAAA |
| MOTA | 712 | CB | ILE A | | 31.817 | 26.932 | | 1.00 26.34 | AAAA |
| ATOM | 713 | CG2 | ILE A | 88 | 32.684 | 27.994 | 36.986 | | AAAA |
| ATOM | 714 | CG1 | ILE A | 88 | 32.354 | 26.543 | 39.026 | 1.00 28.35 | AAAA |
| ATOM | 715 | | ILE A | | 32.356 | 27.671 | 40.042 | 1.00 27.78 | |
| ATOM | 716 | C | ILE A | | 29.946 | 28.110 | 36.472 | 1.00 29.17 | AAAA |
| | 717 | õ | ILE A | | 29.530 | 27.469 | 35.515 | 1.00 29.75 | AAAA |
| MOTA | 718 | N | GLY A | | 30.092 | 29.429 | 36.443 | 1.00 29.96 | AAAA |
| ATOM | | CA | GLY A | | 29.791 | 30.162 | 35.229 | 1.00 30.24 | AAAA |
| ATOM | 719 | | | | 28.430 | | 35.242 | 1.00 30.44 | AAAA |
| ATOM | 720 | C | GLY A | | 28.177 | 31.769 | | 1.00 31.14 | AAAA |
| MOTA | 721 | 0 | GLY A | | 27.542 | 30.268 | | | AAAA |
| MOTA | 722 | N | GLY A | | 26.221 | 30.841 | | | AAAA |
| ATOM | 723 | CA | GLY A | | 26.283 | 32.262 | | | AAAA |
| ATOM | 724 | С | GLY A | | | | | | AAAA |
| . ATCM | ⁻ 25 | 0 | GLY A | | 27.356 | 32.795 | | | AAAA |
| TOM | 726 | N | TYR A | 91 | 25.112 | 32.873 | 30.700 | 1.00 54.05 | |

| | | | | | | 04 077 | 24 212 | 37.290 | 1.00 31.27 | AAAA |
|------|-----|-----|-------|------|---|--------|--------|--------|------------|--------|
| MOTA | 727 | CA | TYR A | 91 | | 24.977 | 34.213 | | - | AAAA |
| ATOM | 728 | CB | TYR A | 91 | | 23.515 | 34.634 | 37.195 | 1.00 31.82 | |
| ATOM | 729 | CG | TYR A | 91 | | 23.169 | 35.825 | 38.047 | 1.00 31.81 | AAAA |
| | 730 | | TYR A | 91 | | 23.536 | 37.108 | 37.670 | 1.00 32.44 | AAAA |
| MOTA | | | | 91 | | 23.250 | 38.203 | 38.475 | 1.00 31.88 | AAAA |
| MOTA | 731 | | TYR A | | | 22.505 | 35.663 | 39.254 | 1.00 32.63 | AAAA |
| MOTA | 732 | | TYR A | 91 | | | 36.754 | 40.068 | 1.00 32.60 | AAAA |
| MOTA | 733 | CE2 | TYR A | 91 | | 22.215 | | | 1.00 31.59 | AAAA |
| ATOM | 734 | CZ | TYR A | 91 | | 22.589 | 38.016 | 39.668 | | |
| ATOM | 735 | OH | TYR A | 91 | | 22.283 | 39.094 | 40.450 | 1.00 31.94 | AAAA |
| | 736 | C | TYR A | 91 | | 25.384 | 34.202 | 38.753 | 1.00 31.56 | AAAA |
| MOTA | | | TYR A | 91 | | 26.075 | 35.105 | 39.233 | 1.00 31.21 | AAAA |
| MOTA | 737 | 0 | | | | 24.925 | 33.158 | 39.438 | 1.00 31.51 | AAAA |
| ATOM | 738 | | GLU A | | | | 32.941 | 40.865 | 1.00 32.70 | AAAA |
| ATOM | 739 | ÇA | GLU A | | | 25.143 | | 41.268 | 1.00 33.55 | AAAA |
| ATOM | 740 | CB | GLU A | | | 24.463 | 31.626 | | 1.00 33.35 | AAAA |
| ATOM | 741 | CG | GLU A | 92 | | 24.174 | 31.495 | 42.747 | | AAAA |
| ATOM | 742 | CD | GLU A | 92 | | 23.311 | 30.278 | 43.087 | 1.00 35.31 | |
| | 743 | | GLU A | | | 23.857 | 29.148 | 43.152 | 1.00 34.30 | AAAA |
| MOTA | 744 | | GLU A | | | 22.076 | 30.466 | 43.275 | 1.00 35.36 | AAAA |
| MOTA | | | | | | 26.619 | 32.902 | 41.248 | 1.00 33.02 | AAAA |
| MOTA | 745 | С | GLU A | | | 27.073 | 33.623 | 42.140 | 1.00 32.91 | AAAA |
| MOTA | 746 | 0 | GLU A | | | | | 40.550 | 1.00 32.84 | AAAA |
| MOTA | 747 | N | ASN A | . 93 | | 27.358 | 32.049 | | 1.00 31.92 | AAAA |
| ATOM | 748 | CA | ASN A | 93 | | 28.785 | 31.861 | 40.777 | | |
| MOTA | 749 | C3 | ASN A | 93 | | 29.015 | 30.437 | 41.278 | 1.00 31.18 | AAAA |
| | 750 | | ASN A | | | 27.948 | 29.994 | 42.259 | 1.00 30.34 | AAAA |
| MOTA | | 001 | ASN A | | | 27.723 | 30.642 | 43.271 | 1.00 31.20 | AAAA |
| ATOM | 751 | | | | | 27.284 | 28.892 | 41.955 | 1.00 29.02 | AAAA |
| MOTA | 752 | | ASN A | | | | 32.052 | 39.411 | 1.00 30.84 | AAAA |
| ATOM | 753 | С | ASN A | | | 29.442 | | 38.758 | 1.00 30.82 | AAAA |
| ATOM | 754 | 0 | ASN A | 93 | | 29.823 | 31.082 | | 1.00 30.52 | AAAA |
| ATOM | 755 | N | PRO A | 94 | | 29.605 | 33.309 | 38.975 | | AAAA |
| ATOM | 756 | CD | PRO A | 94 | | 29.312 | 34.590 | 39.626 | 1.00 29.03 | |
| | 757 | CA | PRO A | | | 30.209 | 33.564 | 37.671 | 1.00 28.89 | AAAA |
| MOTA | | | PRO F | | | 29.890 | 35.045 | 37.416 | 1.00 28.22 | AAAA |
| ATOM | 758 | СЗ | | | | 28.839 | 35.377 | 38.435 | 1.00 29.50 | AAAA |
| MOTA | 759 | CG | PRO A | | | 31.698 | 33.351 | 37.664 | 1.00 28.25 | AAAA |
| ATOM | 760 | C | PRO A | | • | | 32.996 | 38.671 | 1.00 28.21 | AAAA |
| ATOM | 761 | 0 | PRO A | | | 32.308 | | 36.488 | 1.00 27.36 | AAAA |
| ATOM | 762 | N | VAL A | 4 95 | | 32.257 | 33.593 | | 1.00 27.38 | AAAA |
| ATOM | 763 | CA | VAL A | A 95 | | 33.676 | 33.530 | 36.247 | | AAAA |
| ATOM | 764 | CЗ | VAL A | 95 | | 33.945 | 33.289 | 34.741 | 1.00 26.10 | |
| | 765 | | VAL A | | | 35.373 | 33.717 | 34.357 | 1.00 25.47 | AAAA |
| ATOM | 766 | | | | | 33.736 | 31.826 | 34.434 | 1.00 25.59 | AAAA |
| MOTA | | | | | | 34.178 | 34.919 | 36.647 | 1.00 26.56 | AAAA |
| MOTA | 767 | C | VAL | _ | | 33.560 | 35.937 | 36.307 | 1.00 27.18 | AAAA |
| MOTA | 768 | 0 | VAL A | | | | 34.966 | 37.382 | 1.00 25.23 | AAAA |
| MOTA | 769 | N | SER 2 | | | 35.280 | | 37.790 | 1.00 24.51 | AAAA |
| MOTA | 770 | CA | SER A | A 96 | | 35.858 | 36.237 | | | ·AAAA |
| ATOM | 771 | CВ | SER A | A 96 | | 34.935 | 36.961 | 38.774 | | |
| | 772 | OG | SER A | A 96 | | 34.941 | 36.297 | 40.014 | 1.00 19.76 | AAAA |
| ATOM | 773 | c | SER | | | 37.169 | 35.920 | 38.485 | 1.00 24.84 | AAAA |
| ATOM | | 0 | SER | | | 37.590 | 34.764 | 38.530 | 1.00 25.97 | AAAA |
| MOTA | 774 | | | | | 37.824 | 36.933 | 39.030 | 1.00 24.02 | AAAA |
| ATOM | 775 | N | TYR A | | | 39.047 | 36.664 | 39.744 | 1.00 24.55 | AAAA |
| ATOM | 776 | CA | TYR . | | | | 37.762 | 39.504 | 1.00 23.94 | AAAA |
| MOTA | 777 | CB | TYR . | | | 40.071 | 37.702 | | 1.00 23.72 | AAAA |
| ATOM | 778 | CG | TYR . | a 97 | | 40.682 | 37.636 | 38.128 | | AAAA |
| ATOM | 779 | CD1 | | | | 40.177 | 38.341 | 37.039 | 1.00 23.11 | |
| | 780 | C#1 | TYR | | | 40.700 | 38.136 | 35.758 | 1.00 23.50 | AAAA |
| ATOM | | | | | | 41.717 | 36.735 | 37.903 | 1.00 22.25 | AAAA |
| MOTA | 781 | CD2 | | - | | 42.236 | 36.526 | 36.640 | 1.00 22.86 | AAAA |
| ATOM | 782 | CE2 | | | | 41.730 | 37.217 | 35.572 | 1.00 23.56 | AAAA |
| ATOM | 783 | CI | TYR | | | | 36.941 | 34.318 | 1.00 24.06 | AAAA |
| ATOM | 784 | CH | TYR | | | 42.232 | 30.341 | | 1.00 25.08 | AAAA |
| MOTA | 785 | C | TYR | A 97 | | 38.800 | 36.436 | | 1 00 25.00 | AAAA |
| | 786 | Ö | TYR | | | 39.739 | 36.266 | | 1.00 26.91 | |
| MOTA | 787 | N | ALA | | | 37.522 | 36.406 | 41.589 | 1.00 24.73 | AAAA |
| ATCM | | | | _ | | 37.083 | 36.159 | | 1.00 24.50 | AAAA |
| ATOM | 788 | CA | ALA | | | 35.800 | 36.925 | | 1.00 24.48 | AAAA |
| ATOM | 789 | CB | ALA | | | | 34.661 | | 1.00 23.95 | AAAA |
| ATCM | 790 | C | ALA | | | 36.824 | | | 1.00 24.21 | AAAA |
| ATOM | 791 | 0 | ALA | A 98 | | 36.929 | | | | AAAA |
| ATOM | 792 | И | MET | A 99 | | 36.502 | 34.011 | 41.976 | 1.00 43.10 | LUM B. |
| 3100 | | | | | | | | | | • |

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| | | | | 42.000 | 1.00 22.61 | AAAA |
|--------|-------------------|--------|--------|----------|------------|--------|
| ATOM | 793 CA MET A 99 | | 32.584 | 42.000 | 1.00 23.25 | AAAA |
| ATOM | 794 CB MET A 99 | 35.855 | 32.089 | | | |
| | 795 CG MET A 99 | 37.009 | 32.063 | 39.607 | 1.00 23.22 | AAAA |
| ATOM | | | 31.808 | 37.952 | 1.00 25.21 | AAAA |
| MOTA | ,,,, | | 30.374 | 38.258 | 1.00 22.04 | AAAA |
| ATOM | 797 CE MET A 99 | | 31.720 | 42.581 | 1.00 21.80 | AAAA |
| ATOM | 798 C MET A 99 | - | | | 1.00 21.29 | AAAA |
| MOTA | 799 O MET A 99 | | 30.695 | 43.199 | | AAAA |
| | 800 N PHE A 100 | 38.567 | 32.111 | 42.380 | 1.00 21.87 | |
| MOTA | | 39.650 | 31.322 | 42.936 | 1.00 21.11 | AAAA |
| ATOM | | 40.388 | 30.552 | 41.841 | 1.00 20.25 | AAAA |
| ATOM | | 41.451 | 29.648 | 42.375 | 1.00 20.14 | AAAA |
| MOTA | 803 CG PHE A 100 | | | 43.010 | 1.00 20.49 | AAAA |
| ATOM | 804 CD1 PHE A 100 | 41.114 | 28.462 | 42.373 | 1.00 19.82 | AAAA |
| ATOM | 805 CD2 PHE A 100 | 42.785 | 30.050 | | 1.00 19.54 | AAAA |
| ATOM | 806 CE1 PHE A 100 | 42.090 | 27.695 | 43.646 | | AAAA |
| | 807 CE2 PHE A 100 | 43.755 | 29.300 | 43.001 | 1.00 19.22 | |
| MOTA | | 43.410 | 28.122 | 43.641 | 1.00 19.47 | AAAA |
| ATOM | | 40.649 | 32.161 | 43.743 | 1.00 21.37 | AAAA |
| MOTA | 809 C PHE A 100 | 40.959 | 31.822 | 44.887 | 1.00 21.26 | AAAA |
| ATOM | 810 O PHE A 100 | | | 43.161 | 1.00 20.94 | AAAA |
| MOTA | 811 N THR A 101 | 41.142 | 33.252 | | 1.00 21.95 | AAAA |
| ATOM | 812 CA THR A 101 | 42.119 | 34.097 | 43.847 | 1.00 22.21 | AAAA |
| | 813 CB THR A 101 | 42.691 | 35.181 | 42.905 | | |
| MOTA | | 43.511 | 34.552 | 41.917 | 1.00 22.90 | AAAA |
| ATOM | | 43.535 | 36.186 | 43.667 | 1.00 21.38 | AAAA |
| ATOM | | 41.584 | 34.755 | 45.117 | 1.00 22.60 | AAAA |
| MOTA | 816 C THR A 101 | | 34.723 | 46.147 | 1.00 23.38 | AAAA |
| ATOM | 817 O THR A 101 | 42.248 | | 45.049 | 1.00 22.13 | AAAA |
| ATOM | 818 N GLY A 102 | 40.394 | 35.343 | | 1.00 22.03 | AAAA |
| ATOM | 819 CA GLY A 102 | 39.826 | 35.972 | 46.227 | | AAAA |
| | 820 C GLY A 102 | 39.340 | 34.928 | 47.221 | 1.00 21.36 | |
| MOTA | | 39.433 | 35.104 | 48.439 | 1.00 20.02 | AAAA |
| ATOM | | 38.816 | 33.833 | 46.677 | 1.00 21.86 | AAAA |
| MOTA | 822 N SER A 103 | 38.311 | 32.719 | 47.466 | 1.00 21.68 | AAAA |
| MOTA | 823 CA SER A 103 | | 31.668 | 46.557 | 1.00 21.56 | AAAA |
| MOTA | 824 CB SER A 103 | 37.699 | | | 1.00 23.67 | AAAA |
| ATOM | 825 OG SER A 103 | 36.604 | 32.216 | 45.857 | 1.00 23.67 | AAAA |
| | 826 C SER A 103 | 39.450 | 32.098 | 48.229 | | AAAA |
| ATOM | 827 O SER A 103 | 39.314 | 31.806 | 49.412. | 1.00 22.44 | |
| ATOM | | 40.578 | 31.898 | 47.545 | 1.00 23.37 | AAAA |
| MOTA | | 41.746 | 31.305 | 48.183 | 1.00 23.50 | AAAA |
| ATOM | 829 CA SER A 104 | | 31.070 | 47.172 | 1.00 24.80 | AAAA |
| ATOM | 830 CB SER A 104 | 42.862 | 30.169 | 46.175 | 1.00 28.38 | AAAA |
| ATOM | 831 OG SER A 104 | 42.441 | | 49.256 | 1.00 22.79 | AAAA |
| ATOM | 832 C SER A 104 | 42.254 | 32.230 | | 1.00 22.66 | AAAA |
| ATOM | 833 O SER A 104 | 42.707 | 31.794 | 50.307 | 1.00 22.00 | AAAA |
| | 834 N LEU A 105 | 42.160 | 33.518 | 48.970 | 1.00 22.08 | |
| ATOM | | 42.626 | 34.541 | 49.870 | 1.00 21.70 | AAAA |
| MOTA | | 42.524 | 35.882 | | 1.00 21.89 | AAAA |
| ATOM | 836 CB LEU A 105 | 43.332 | 37.038 | | 1.00 23.64 | AAAA |
| ATOM | 837 CG LEU A 105 | | 36.692 | | 1.00 22.01 | AAAA |
| ATOM | 838 CD1 LEU A 105 | 44.830 | 30.094 | | 1.00 23.60 | AAAA |
| ATOM | 839 CD2 LEU A 105 | 43.004 | 38.304 | | 1.00 22.29 | AAAA |
| ATOM | 840 C LEU A 105 | 41.767 | 34.525 | 51.131 | 1.00 22.25 | AAAA |
| | 841 O LEU A 105 | 42.277 | 34.595 | 52.249 | 1.00 21.95 | |
| atom | | 40.458 | 34.429 | 50.934 | 1.00 22.23 | AAAA |
| MOTA | | 39.515 | 34.394 | 52.042 | 1.00 22.32 | AAAA |
| ATOM | 843 CA ALA A 106 | 38.068 | 34.472 | | | Aaaa |
| MOTA | 844 CB ALA A 106 | | 33.126 | | | AAAA |
| ATOM | 845 C ALA A 106 | 39.704 | | | | AAAA |
| ATOM | 846 O ALA A 106 | 39.578 | 33.145 | | | AAAA |
| ATOM | 847 N THR A 107 | 40.011 | 32.032 | | | AAAA |
| | 848 CA THR A 107 | 40.209 | 30.732 | | | |
| MOTA | | 40.170 | 29.571 | 51.749 | 1.00 19.82 | AAAA |
| MOTA | | 38.903 | 29.553 | | 1.00 18.56 | АААА |
| MOTA | 850 OG1 THR A 107 | | 28.242 | | | AAAA |
| ATOM | 851 CG2 THR A 107 | 40.360 | | | | AAAA |
| ATOM | 852 C THR A 107 | 41.516 | 30.630 | | | AAAA |
| | 853 O THR A 107 | 41.537 | 30.040 | | | AAAA |
| ATOM | 854 N GLY A 108 | 42.601 | 31.176 | | | |
| ATOM | | 43.878 | 31.14 | 5 53.684 | 1.00 18.20 | АААА |
| ATOM | | 43.739 | 31.93 | | 1.00 18.43 | Алла |
| ATOM - | 856 C GLY A 108 | | 31.600 | | | AAAA |
| ATOM | 857 O GLY A 108 | 44.335 | | | | , AAAA |
| ATOM | 858 N SER A 109 | 42.909 | 32.96 | , ,4.,4. | | • |
| | | | | | | |

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| • | | J | | | | |
|--------|-----------------------------------|--------|---------------------|----------|------------|-------|
| | 100 | 42.683 | 33.805 | 56.098 | 1.00 19.67 | AAAA |
| MOTA | 859 CA SER A 109 | | 35.058 | 55.707 | 1.00 20.27 | AAAA |
| ATOM | 860 CB SER A 109 | | | | 1.00 21.80 | AAAA |
| ATOM | 861 OG SER A 109 | | 35.803 | | | AAAA |
| | 862 C SER A 109 | 41.955 | 33.066 | 57.219 | 1.00 19.61 | |
| MOTA | | 42.078 | 33.426 | 58.388 | 1.00 18.40 | AAAA |
| ATOM | | | 32.042 | 56.866 | 1.00 19.88 | AAAA |
| ATOM - | 864 N THR A 110 | | 31.288 | 57.891 | 1.00 20.51 | AAAA |
| MOTA | 865 CA THR A 110 | | | 57.001 | 1.00 20.62 | ÄAAA |
| | 866 CB THR A 110 | 39.365 | 30.438 | 57.304 | | AAAA |
| ATOM | | 38.236 | 31.284 | 57.050 | 1.00 20.80 | • |
| MOTA | | 38.974 | 29.313 | 58.262 | 1.00 20.53 | AAAA |
| ATOM | · · · · · · · · · · · · · · · · · | 41.504 | 30.420 | 58.601 | 1.00 20.36 | AAAA |
| ATOM | 869 C THR A 110 | | 30.268 | 59.822 | 1.00 20.78 | AAAA |
| MOTA | 870 O THR A 110 | 41.455 | _ | | 1.00 20.85 | AAAA |
| ATOM | 871 N VAL A 111 | 42.431 | 29.855 | 57.832 | 1.00 20.03 | AAAA |
| | 872 CA VAL A 111 | 43.480 | 29.053 | 58.423 | | |
| ATOM | | 44.318 | 28.323 | 57.345 | 1.00 21.05 | AAAA |
| MOTA | | 45.537 | 27.644 | 57.983 | 1.00 19.91 | -AAAA |
| MOTA | 874 CG1 VAL A 111 | 43.460 | 27.281 | 56.648 | 1.00 18.39 | AAAA |
| MOTA | 875 CG2 VAL A 111 | | | 59.232 | 1.00 21.84 | AAAA |
| ATOM | 876 C VAL A 111 | 44.374 | 30.005 | - | 1.00 22.73 | AAAA |
| | 877 O VAL A 111 | 44.825 | 29.671 | 60.331 | 1.00 22.73 | AAAA |
| MOTA | 878 N GLN A 112 | 44.612 | 31.204 | 58.712 | 1.00 21.62 | |
| MOTA | | 45.449 | 32.133 | 59.452 | 1.00 21.89 | AAAA |
| MOTA | | 45.630 | 33.450 | 58.690 | 1.00 22.50 | AAAA |
| ATOM | 880 CB GLN A 112 | | 33.283 | 57.335 | 1.00 23.68 | AAAA |
| ATOM | 881 CG GLN A 112 | 46.288 | | _ | 1.00 23.18 | AAAA |
| ATOM | 882 CD GLN A 112 | 46.414 | 34.578 | 56.569 | | AAAA |
| | 883 OE1 GLN A 112 | 47.389 | 35.310 | 56.722 | 1.00 23.86 | |
| MOTA | | 45.413 | 34.879 | 55.752 | 1.00 21.90 | AAAA |
| MOTA | | 44.766 | 32.383 | 60.774 | 1.00 21.84 | AAAA |
| ATCM | 885 C GLN A 112 | 45.389 | 32.316 | 61.835 | 1.00 22.47 | AAAA |
| ATOM | 886 O GLN A 112 | | | 60.700 | 1.00 21.34 | AAAA |
| ATOM | 887 N ALA A 113 | 43.468 | 32.651 | | 1.00 20.84 | AAAA |
| ATOM | 888 CA ALA A 113 | 42.682 | 32.934 | 61.884 | 1.00 18.52 | AAAA |
| | 889 CB ALA A 113 | 41.244 | 33.172 | 61.504 | 1.00 18.52 | |
| MOTA | | 42.795 | 31.782 | 62.865 | 1.00 21.75 | AAAA |
| ATOM | 413 | 42.880 | 31.985 | 64.084 | 1.00 22.24 | AAAA |
| MOTA | | 42.797 | 30.569 | 62.329 | 1.00 22.54 | AAAA |
| ATOM | 892 N ILE A 114 | | 29.393 | 63.160 | 1.00 23.16 | AAAA |
| ATOM | 893 CA ILE A 114 | 42.891 | | 62.352 | 1.00 23.33 | AAAA |
| ATOM | 894 CB ILE A 114 | 42.557 | 28.146 | | 1.00 23.80 | AAAA |
| | 895 CG2 ILE A 114 | 42.939 | 26.912 | 63.106 | | AAAA |
| ATOM | | 41.058 | 28.130 | 62.047 | 1.00 23.48 | |
| ATOM | | 40.610 | 26.951 | 61.204 | 1.00 22.08 | AAAA |
| MOTA | | 44.268 | 29.270 | 63.792 | 1.00 24.33 | AAAA |
| MOTA | 898 C ILE A 114 | | 29.013 | 64.990 | 1.00 25.30 | AAAA |
| ATCM | 899 O ILE A 114 | 44.373 | | 63.002 | 1.00 24.96 | AAAA |
| ATOM | 900 N GLU A 115 | 45.319 | 29.490 | | 1.00 26.61 | AAAA |
| | 901 CA GLU A 115 | 46.699 | 29.395 | 63.503 | | AAAA |
| MOTA | 902 CB GLU A 115 | 47.708 | 29.753 | 62.406 | 1.00 24.75 | |
| atom | | 47.444 | 29.033 | 61.103 | 1.00 25.80 | AAAA |
| ATOM | | 48.471 | 29.323 | 60.030 | 1.00 26.07 | AAAA |
| ATCM | 904 CD GLU A 115 | | 30.484 | | 1.00 27.15 | AAAA |
| MOTA | 905 OE1 GLU A 115 | 48.911 | | | 1.00 25.45 | AAAA |
| MOTA | 906 OE2 GLU A 115 | 48.819 | 28.402 | | 1.00 27.89 | AAAA |
| ATOM | 907 C GLU A 115 | 46.877 | 30.340 | | | AAAA |
| | 908 O GLU A 115 | 47.480 | 29. 9 75 | 65.695 | 1.00 28.04 | |
| ATOM | | 46.337 | 31.552 | .64.531 | 1.00 29.15 | AAAA |
| MOTA | | 46.408 | 32.579 | | 1.00 29.42 | AAAA |
| MOTA | 910 CA GLU A 116 | | 33.871 | | 1.00 28.26 | AAAA |
| ATOM | 911 CB GLU A 116 | 45.751 | | | 1.00 28.93 | AAAA |
| ATOM | 912 CG GLU A 116 | 46.482 | 34.529 | | | AAAA |
| | 913 CD GLU A 116 | 47.902 | 34.937 | 64.318 | | AAAA |
| MOTA | | 48.081 | 35.878 | 65.123 | 1.00 27.68 | |
| atom | | 48.838 | 34.297 | 63.810 | 1.00 27.38 | AAAA |
| ATOM | 915 OE2 GLU A 116 | 45.737 | | | 1.00 29.77 | AAAA |
| ATOM | 916 C GLU A 116 | | | | | AAAA |
| ATOM | 917 O GLU A 116 | 46.338 | | | | AAAA |
| | 918 N PHE A 117 | 44.492 | | | | AAAA |
| ATCM | | 43,741 | 31.204 | | 1.00 29.33 | |
| ATOM | | 42.425 | | 67.480 | 1.00 28.89 | AAAA |
| ATOM | | 41.604 | | | 1.00 28.93 | AAAA |
| ATOM | 921 CG PHE A 117 | | | _ • | | AAAA |
| ATOM | 922 CD1 PHE A 117 | 41.010 | | · | | AAAA |
| ATCM | 923 CD2 PHE A 117 | 41.441 | 28.72 | | | AAAA |
| | 924 CE1 PHE A 117 | 40.261 | 30.58 | g 70.610 | 1.00 20.00 | |
| ATOM | 724 VIII | | | | | |
| | | | | | | |

| | | | | | . ` | | | | | |
|--------------|--------------------|-----------|-------|----------------|-----|------------------|------------------|------------------|--------------------------|--------------|
| . = | 025 | CE2 | PHE A | 117 | | 40.695 | 28.284 | 70.009 | 1.00 29.16 | AAAA |
| ATOM | 925 926 | | PHE A | | | 40.103 | 29.227 | 70.862 | 1.00 29.03 | AAAA |
| ATOM ATOM | 927 | | PHE A | | | 44.545 | 30.195 | 68.671 | 1.00 29.22 | AAAA |
| ATOM | 928 | | PHE A | | | 44.677 | 30.315 | 69.884 | 1.00 30.29 | AAAA |
| ATOM | 929 | | LEU A | | | 45.066 | 29.195 | 67.965 | 1.00 29.24 | AAAA |
| ATOM | 930 | | LEU A | | | 45.864 | 28.145 | 68.576 | 1.00 29.50 | AAAA AAAA |
| ATOM | 931 | CB | LEU A | 118 | | 46.182 | 27.047 | 67.550 | 1.00 28.57 | AAAA AAAA |
| ATOM | 932 | | LEU A | | • | 44.962 | 26.296 | 66.989 | 1.00 28.16 1.00 25.58 | AAAA |
| ATOM | 933 | | LEU A | | | 45.421 | 25.090 | 66.191 68.128 | 1.00 25.58 | AAAA |
| MOTA | 934 | | LEU A | | | 44.053 | 25.846 | 69.227 | 1.00 27.04 | AAAA |
| ATOM | 935 | С | LEU A | | | 47.150 | 28.649 | 70.056 | 1.00 30.14 | AAAA |
| MOTA | 936 | 0 | LEU A | | | 47.727 47.602 | 27.954 29.845 | 68.847 | 1.00 31.36 | AAAA |
| ATOM | 937 | N | LYS A | | | 47.602 | 30.451 | 69.448 | 1.00 32.52 | AAAA |
| MOTA | 938 | CA | LYS A | | | 49.396 | 31.539 | 68.559 | 1.00 32.38 | AAAA |
| ATOM | 939 | CB | LYS A | | | 49.882 | 31.108 | 67.199 | 1.00 33.03 | AAAA |
| MOTA | 940 | CG | LYS A | | | 50.371 | 32.321 | 66.411 | 1.00 32.74 | AAAA |
| ATOM | 941 942 | CD CE | LYS ? | | | 50.681 | 31.939 | 64.972 | 1.00 33.94 | AAAA |
| ATOM | 942 | NZ | LYS A | | | 51.125 | 33.099 | 64.152 | 1.00 34.93 | AAAA |
| MOTA | 944 | C | LYS ? | | | 48.385 | 31.143 | 70.744 | 1.00 33.74 | AAAA |
| MOTA MOTA | 945 | o | LYS A | 119 | | 49.218 | 31.748 | 71.413 | 1.00 34.85 | AAAA |
| ATOM | 946 | N | GLY A | | | 47.096 | 31.079 | 71.073 | 1.00 33.68 | AAAA |
| ATOM | 947 | CA | GLY A | | | 46.600 | 31.736 | 72.263 | 1.00 33.69 | AAAA |
| ATOM | 948 | С | GLY A | 120 | | 45.987 | 33.110 | 71.988 | 1.00 34.11 | AAAA AAAA |
| ATOM | 949 | 0 | GLY 2 | | | 45.588 | 33.802 | 72.932 | 1.00 33.65 | AAAA |
| ATOM | 950 | \cdot N | ASN A | | | 45.904 | 33.513 | 70.717 70.368 | 1.00 33.58 1.00 33.35 | AAAA |
| MOTA | 951 | CA | ASN A | 121 | | 45.326 | 34.820 | 69.341 | 1.00 33.33 | AAAA |
| ATOM | 952 | CB | ASN A | | • | 46.194 | 35.537 35.828 | 69.859 | 1.00 34.31 | AAAA |
| MOTA | 953 | CG | ASN A | | | 47.570 48.333 | 34.921 | 70.154 | | AAAA |
| ATOM | 954 | | ASN A | | | 40.333 | 37.096 | 69.975 | 1.00 34.18 | AAAA |
| ATOM | 955 | | ASN A | | | 43.888 | 34.805 | 69.839 | 1.00 32.85 | AAAA |
| ATOM | 956 | C | | A 121 | | 43.304 | 33.751 | 69.599 | 1.00 32.78 | AAAA |
| ATOM | 957 | 0 | | A 121 | | 43.338 | 36.003 | 69.655 | 1.00 32.47 | AAAA |
| ATOM | 958 95 9 | N CA | | A 122 | | 41.980 | 36.200 | 69.148 | 1.00 30.89 | AAAA |
| ATOM | 960 | CB | | A 122 | | 41.182 | 37.145 | 70.070 | 1.00 31.05 | AAAA |
| MOTA MOTA | 961 | | VAL | | | 39.831 | 37.423 | 69.489 | 1.00 30.95 | AAAA |
| ATOM | 962 | | VAL : | | | 41.038 | 36.516 | 71.440 | 1.00 31.19 | AAAA |
| ATOM | 963 | С | | A 122 | | 42.056 | 36.805 | 67.750 | 1.00 30.19 | AAAA AAAA |
| ATOM . | 964 | 0 | | A 122 | | 42.694 | 37.840 | 67.535 | 1.00 31.28 1.00 28.62 | AAAA |
| ATOM | 965 | N | | A 123 | | 41.405 | 36.147 | 66.800 | 1.00 28.62 1.00 26.49 | AAAA |
| ATOM | 966 | CA | | A 123 | | 41.415 | 36.589 | 65.421 64.599 | 1.00 26.51 | AAAA |
| MOTA . | 967 | CB | | A 123 | | 42.323 | 35.708 36.570 | 64.836 | 1.00 25.59 | AAAA |
| ATOM | 968 | С | | A 123 | | 40.038 | 35.814 | 65.252 | 1.00 26.27 | AAAA |
| MOTA | 969 | 0 | | A 123 | | 39.173 39.848 | 37.421 | 62.847 | 1.00 25.44 | AAAA |
| MOTA | 970 | N | | A 124 | | 38.590 | 37.534 | 62.156 | 1.00 23.87 | AAAA |
| MOTA | 971 | CA | PHE. | A 124 A 124 | | 37.832 | 38.779 | 63.646 | 1.00 23.58 | AAAA |
| ATOM | 972 | CB | | A 124 | | 36.591 | 39.119 | 62.841 | 1.00 23.71 | AAAA |
| ATOM | 973 974 | CG | PHE | | | 35.668 | 38.140 | 62.495 | 1.00 23.44 | AAAA |
| ATOM | 975 | | PHE | | | 36.311 | 40.449 | 62.498 | 1.00 23.75 | AAAA |
| ATOM | 976 | CE1 | PHE | A 124 | | 34.479 | 38.483 | 61.823 | 1.00 23.31 | AAAA |
| ATOM ATOM | 977 | | PHE | | | 35.131 | 40.796 | 61.833 | 1.00 21.71 | AAAA |
| ATOM | 978 | CZ | | A 124 | | 34.217 | 39.815 | 61.497 | 1.00 22.35 | AAAA |
| ATOM | 979 | c | | A 124 | | 38.951 | 37.673 | 61.700 | 1.00 23.26 | AAAA AAAA |
| ATCM | 980 | ō | | Á 124 | | 39.720 | 38.555 | 61.323 | 1.00 22.29 | |
| ATOM | 981 | N | ASN | A 125 | | 38.427 | 36.759 | 60.897 | 1.00 23.24 | AAAA AAAA |
| ATOM | 982 | CA | ASN | A 125 | | 38.622 | 36.785 | 59:457 | 1.00 21.08 1.00 19.90 | AAAA |
| ATOM | 983 | СВ | ASN | A 125 | | 39.181 | 35.470 | 58.951 | 1.00 19.90 | AAAA |
| ATOM | 984 | CG | ASN | A 125 | | 39.098 | 35.360 | 57.454 | 1.00 20.64 | AAAA |
| ATOM | 285 | | | A 125 | | 39.389 | 36.317 | 56.748 56.956 | 1.00 19.93 | AAAA |
| ATOM | 986 | ND2 | | A 125 | | 38.721 | 34.190 | 58.813 | | AAAA |
| ATOM | 987 | С | | A 125 | | 37.269 | 37.059 36.148 | | | AAAA |
| ATOM | 588 | 0 | ASN | A 125 | | 36.469 | 38.340 | | | AAAA |
| ATOM | 989 | N | PRO | A 126 | | 36.991 | | | | AAAA |
| ATOM | 990 | CD | PRO | A 126 | | 37.893 | JJ.40U | | | |

| | | | | 5 | | | | | | |
|--------------|--------------|----------|------------------------|-----|------------------|------------------|------------------|--------|----------------|----------------|
| | | | nno n 126 | | 35.766 | 38.849 | 57.932 | 1.00 1 | 9.52 | AAAA |
| ATOM | | CA | PRO A 126 PRO A 126 | | 36.005 | 40.359 | 57.941 | 1.00 1 | 8.55 | AAAA |
| MOTA | - | CB | PRO A 126 | | 37.511 | 40.465 | 57.799 | 1.00 1 | | AAAA |
| MOTA | 993 | | PRO A 126 | | 35.456 | 38.313 | 56.526 | 1.00 1 | | AAAA |
| ATOM | 994 | | PRO A 126 | | 34.303 | 38.349 | 56.080 | 1.00 1 | | AAAA |
| MOTA | 995 | | ALA A 12 | | 36.477 | 37.814 | 55.835 | 1.00 1 | 8.17 | AAAA |
| MOTA | 996 | | ALA A 12 | | 36.283 | 37.314 | 54.481 | 1.00 1 | | AAAA |
| MOTA | 997 | | ALA A 12 | | 37.547 | 37.520 | 53.658 | 1.00 1 | 7.08 | AAAA |
| MOTA | 998 | CB | ALA A 12 | | 35.875 | 35.857 | 54.443 | 1.00 1 | | AAAA |
| ATOM | 999 | C | ALA A 12 | | 35.438 | 35.359 | 53.409 | 1.00 1 | | AAAA |
| MOTA | 1000 | 0 | GLY A 12 | | 36.019 | 35.180 | 55.570 | 1.00 1 | | AAAA |
| MOTA | 1001 | N | GLY A 12 | | 35.685 | 33.780 | 55.642 | 1.00 1 | | AAAA |
| MOTA | 1002 | CA | GLY A 12 | - | 34.226 | 33.593 | 55.955 | 1.00 1 | | AAAA |
| MOTA | 1003 | С 0 | GLY A 12 | | 33.485 | 34.557 | 55.997 | 1.00 1 | | AAAA |
| ATOM | 1004 1005 | N | GLY A 12 | á | 33.821 | 32.353 | 56.198 | 1.00 1 | | AAAA |
| MOTA | 1005 | CA | GLY A 12 | 9 | 32.426 | 32.082 | 56.462 | 1.00 1 | | AAAA |
| MOTA | 1007 | C | GLY A 12 | 9 | 31.669 | 31.822 | 55.169 | 1.00 1 | | AAAA |
| ATOM | 1007 | ō | GLY A 12 | 9 | 30.469 | 32.051 | 55.108 | 1.00 1 | | - AAAA AAAA |
| MOTA | 1009 | N | MET A 13 | 0 | 32.380 | 31.368 | 54.137 | 1.00 2 | | AAAA AAAA |
| MOTA MOTA | 1010 | CA | MET A 13 | 0 | 31.790 | 31.029 | 52.826 | 1.00 2 | 21.60 | AAAA |
| | 1011 | CB | MET A 13 | 0 | 32.866 | 31.117 | 51.744 | 1.00 2 | 22.02 | AAAA |
| MOTA MOTA | 1012 | CG | MET A 13 | | 33.551 | 32.472 | 51.698 | 1.00 2 | | AAAA |
| ATOM | 1013 | SD | MET A 13 | 0 | 34.971 | 32.567 | 50.599 | 1.00 2 | | AAAA |
| ATOM | 1014 | CE | MET A 13 | 0 | 34.268 | 32.137 | 49.048 | 1.00 2 | | AAAA . |
| ATOM | 1015 | C. | MET A 13 | 0 | 31.328 | 29.587 | 53.002 | 1.00 2 | | AAAA |
| ATOM | 1016 | ō | MET A 13 | 0 | 31.970 | 28.641 | 52.546 | 1.00 2 | 22.30 | AAAA |
| ATOM | 1017 | N | HIS A 13 | | 30.184 | 29.452 | 53.659 | 1.00 | | AAAA |
| ATOM | 1018 | CA | HIS A 13 | 1 | 29.618 | 28.171 | 54.062 | 1.00 | | AAAA |
| ATOM | 1019 | CB | HIS A 13 | 1 | 28.832 | 28.421 | 55.342 | 1.00 | | AAAA |
| ATOM | 1020 | CG | HIS A 13 | 1 | 27.679 | 29.360 | 55.161 | 1.00 | | AAAA |
| ATOM | 1021 | CD2 | HIS A 13 | 1 | 27.091 | 29.846 | 54.043 | 1.00 | 19 33 | AAAA |
| ATOM | 1022 | ND1 | HIS A 13 | 1 | 26.952 | 29.854 | 56.219 55.758 | 1.00 | 16.99 | AAAA |
| ATOM | 1023 | CE1 | HIS A 13 | 1 | 25.968 | 30.607 | 54.441 | 1.00 | | AAAA |
| MOTA | 1024 | NE2 | HIS A 13 | 1 | 26.031 | 30.617 | 53.141 | 1 00 | 19.97 | AAAA |
| ATOM | 1025 | C | HIS A 13 | | 28.763 | 27.332 | 53.541 | 1 00 | 19.61 | AAAA |
| ATOM | 1026 | 0 | HIS A 13 | 1 | 28.330 | 26.262 27.796 | 51.923 | 1.00 | 20.11 | AAAA |
| ATOM | 1027 | N | HIS A 13 | 2 | 28.518 | 27.758 | 50.994 | 1.00 | 17.76 | AAAA |
| MOTA | 1028 | CA | HIS A 1 | 2 | 27.673 | 28.044 | 50.127 | | 16.76 | AAAA |
| MOTA | 1029 | CB | HIS A 1 | 2 | 26.879 25.824 | 28.815 | 50.862 | | 15.35 | AAAA |
| ATOM | 1030 | CG | HIS A 1 | 2 | 25.567 | | 50.920 | 1.00 | 14.15 | AAAA |
| MOTA | 1031 | CD2 | HIS A 1 | 2 | 24.804 | 28.200 | 51.557 | 1.00 | 16.15 | AAAA |
| MOTA | 1032 | ND1 | HIS A 1 | 2 | 23.966 | | 52.005 | 1.00 | 14.13 | AAAA |
| MOTA | 1033 | CEI | HIS A 1 | 12 | 24.405 | | 51.632 | 1.00 | 14.65 | AAAA |
| MOTA | 1034 | NE2 | HIS A 1 | 22 | 28.355 | | 50.065 | | 17.99 | AAAA |
| MOTA | | | HIS A 1 HIS A 1 | 32 | 27.742 | | 49.684 | 1.00 | 18.54 | AAAA |
| MOTA | 1.36 | 0 | ALA A 1 | 12 | 29.604 | | 49.690 | 1.00 | 17.82 | AAAA |
| MOTA | 1.37 | N | ALA A 1 | 33 | 30.300 | | 48.742 | 1.00 | 18.38 | AAAA |
| MOTA | 1038 | CA CB | ALA A 1 | | 31.684 | | | 1.00 | 17.53 | AAAA |
| ATOM | 1039 | C | ALA A 1 | | 30.366 | | | | 20.92 | AAAA |
| ATOM | 1040 1041 | o | ALA A 1 | | 30.578 | | 50.298 | | 21.79 | AAAA |
| ATOM | 1041 | N | PHE A 1 | | 30.184 | 23.086 | | 1.00 | 20.58 | AAAA |
| MOTA | 1042 | CA | PHE A 1 | | 30.258 | 21.663 | 48.455 | 1.00 | 21.38 | AAAA AAAA |
| MOTA | 1043 | CB | PHE A 1 | | 29.168 | 20.860 | | | 19.41 | AAAA |
| ATOM | 1045 | CG | PHE A 1 | 34 | 27.772 | 21.229 | | 1.00 | 18.32 | AAAA |
| MOTA | 1045 | | 1 PHE A 1 | 34 | 27.027 | | | | 19.22 | AAAA |
| MOTA | 1047 | | 2 PHE A 1 | 34 | 27.193 | | | | 19.14 | AAAA |
| MOTA ATOM | 1048 | | 1 PHE A 1 | 34 | 25.714 | | | 1.00 | 18.56 | AAAA |
| MOTA | 1049 | | | | 25.889 | | | | 17.72 | AAAA |
| ATOM | 1050 | | | | 25.158 | | | | 18.01 22.90 | AAAA |
| MOTA | 1051 | | PHE A 1 | | 31.629 | | | | 23.37 | AAAA |
| MOTA | 1052 | | PHE A 1 | | 32.459 | | | | 24.63 | AAAA |
| ATOM | 1053 | | LYS A 1 | 35 | 31.842 | | | | 27.16 | AAAA |
| ATOM | 1054 | | LYS A | 35 | 33.09 | | 48.122 | | 28.53 | AAAA |
| ATOM | 1055 | _ | LYS A 1 | .35 | 32.92 | | | | 31.01 | AAAA |
| ATOM | 1056 | | | .35 | 34.13 | 3 16.84 | 48.292 | . 1.00 | J U. | |
| A.On | | | | | | | | | | |

| | | CD | tve : | A 135 | 33.879 | 15.472 | 48.910 | 1.00 32.75 | AAAA |
|------|------|-----|-------|-------|----------|------------------|--------|------------------------|--------|
| MOTA | 1057 | | | A 135 | 33.961 | 15.495 | 50.457 | 1.00 33.96 | AAAA |
| MOTA | 1058 | | | A 135 | 35.371 | 15.664 | 50.976 | 1.00 33.04 | AAAA |
| ATOM | 1059 | | | A 135 | 33.577 | 19.390 | 46.673 | 1.00 27.37 | AAAA |
| ATOM | 1060 | | | A 135 | 34.769 | 19.596 | 46.437 | 1.00 27.35 | AAAA |
| MOTA | 1061 | | | | 32.658 | 19.354 | 45.714 | 1.00 27.32 | AAAA |
| MOTA | 1062 | | | A 136 | 33.028 | 19.527 | 44.313 | 1.00 28.31 | AAAA |
| MOTA | 1063 | | | A 136 | 33.023 | 18.162 | 43.626 | 1.00 28.56 | AAAA |
| MOTA | 1064 | | | A 136 | 33.822 | 17.242 | 44.417 | 1.00 29.28 | AAAA |
| MOTA | 1065 | | | A 136 | 31.993 | 20.395 | 43.599 | 1.00 28.91 | AAAA |
| MOTA | 1066 | | | A 136 | | 20.080 | 42.486 | 1.00 28.78 | AAAA |
| ATOM | 1067 | 0 | | A 136 | . 31.568 | 21.502 | 44.212 | 1.00 29.08 | AAAA. |
| ATOM | 1068 | | | A 137 | 31.595 | 22.311 | 43.576 | 1.00 29.66 | AAAA |
| MOTA | 1069 | | | A 137 | 30.574 | 21.528 | 43.657 | 1.00 31.65 | AAAA |
| MOTA | 1070 | | | A 137 | 29.259 | 22.273 | 43.355 | 1.00 33.89 | AAAA |
| ATOM | 1071 | | | A 137 | 27.989 | 21.267 | 43.373 | 1.00 35.93 | AAAA |
| MOTA | 1072 | | | A 137 | 26.862 | 20.366 | 42.228 | 1.00 36.31 | AAAA |
| MOTA | 1073 | NE | | A 137 | 26.961 | 20.560 | 41.015 | 1.00 35.99 | AAAA |
| ATOM | 1074 | CZ | | A 137 | 26.505 | 21.834 | 40.798 | 1.00 34.63 | AAAA |
| MOTA | 1075 | | | A 137 | 25.915 | | 40.025 | 1.00 35.35 | AAAA |
| ATOM | 1076 | | ARG . | A 137 | 26.650 | 19.786 23.723 | 44.116 | 1.00 28.53 | AAAA |
| ATOM | 1077 | С | | A 137 | 30.402 | | 45.324 | 1.00 28.51 | AAAA |
| ATOM | 1078 | 0 | | A 137 | 30.418 | 23.946 | 43.202 | 1.00 27.53 | AAAA |
| ATOM | 1079 | N | | A 138 | 30.247 | 24.673 | 43.581 | 1.00 27.64 | AAAA |
| MOTA | 1080 | CA | | A 138 | 30.039 | 26.063 | 42.381 | 1.00 27.87 | AAAA |
| MOTA | 1081 | CB | | A 138 | 30.236 | 26.984 | 44.079 | 1.00 27.27 | AAAA |
| ATOM | 1082 | С | | A 138 | 28.601 | 26.130 | 43.671 | 1.00 28.30 | AAAA |
| MOTA | 1083 | 0 | | A 138 | 27.769 | 25.321 | 44.951 | 1.00 26.16 | AAAA |
| ATOM | 1084 | N | | A 139 | 28.292 | 27.080 | 45.480 | 1.00 25.39 | AAAA |
| MOTA | 1085 | CA | | A 139 | 26.945 | 27.134 | 46.282 | 1.00 24.58 | AAAA |
| ATOM | 1086 | CB | | A 139 | 26.673 | 25.847 | 47.017 | 1.00 25.37 | AAAA |
| ATOM | 1087 | CG | | A 139 | 25.343 | 25.872 | 46.413 | 1.00 24.20 | AAAA |
| ATOM | 1088 | ODl | ASN | A 139 | 24.272 | 26.017 25.720 | 48.338 | 1.00 24.91 | AAAA |
| ATOM | 1089 | | ASN | A 139 | 25.408 | | 46.341 | 1.00 24.90 | AAAA |
| ATOM | 1090 | Ç | ASN | A 139 | . 26.683 | 28.358 | 47.348 | 1.00 24.98 | AAAA |
| ATOM | 1091 | 0 | ASN | A 139 | 27.346 | 28.570 | 45.916 | 1.00 24.46 | AAAA |
| ATOM | 1092 | 11 | | A 140 | 25.702 | 29.145 | 46.625 | 1.00 22.96 | AAAA |
| ATOM | 1093 | ÇA | | A 140 | 25.294 | 30.336 | 46.755 | 1.00 22.24 | AAAA |
| ATOM | 1094 | С | | A 140 | 26.383 | 31.358 | 47.867 | 1.00 23.09 | AAAA |
| ATOM | 1095 | 0 | | A 140 | 26.663 | 31.817 | 45.625 | 1.00 20.60 | AAAA |
| MOTA | 1096 | N | PHE | A 141 | 26.992 | 31.711 | 45.572 | 1.00 19.43 | AAAA |
| MOTA | 1097 | CA | | A 141 | 28.075 | 32.700 33.920 | 46.430 | 1.00 19.86 | AAAA |
| ATOM | 1098 | CB | | A 141 | 27.758 | 34.577 | 46.114 | 1.00 21.18 | AAAA |
| ATOM | 1099 | CG | | A 141 | 26.453 | | 46.934 | 1.00 20.49 | AAAA |
| ATOM | 1100 | | | A 141 | 25.974 | 35.592 | 44.985 | 1.00 21.42 | · AAAA |
| MOTA | 1101 | CD2 | PHE | A 141 | 25.723 | 34.218 | 46.638 | 1.00 22.45 | AAAA |
| MOTA | 1102 | CE1 | PHE | A 141 | 24.800 | 36.242 34.859 | 44.672 | 1.00 :1.76 | AAAA |
| MOTA | 1103 | | | A 141 | 24.540 | 35.881 | 45.499 | 1.00 `3.05 | AAAA |
| ATOM | 1104 | CZ | | A 141 | 24.072 | 32.132 | 46.069 | 1.00 18.68 | AAAA |
| MOTA | 1105 | С | | A 141 | 29.396 | 32.784 | 45.944 | 1.00 19.19 | AAAA |
| ATOM | 1106 | 0 | | A 141 | 30.438 | 30.930 | 46.635 | 1.00 16.93 | AAAA |
| ATOM | 1107 | N | | A 142 | 29.367 | 30.332 | | 1.00 16.80 | AAAA |
| ATOM | 1108 | CA | | A 142 | 30.594 | 29.689 | | 1.00 16.51 | AAAA |
| MOTA | 1109 | CB | | A 142 | 30.323 | 29.009 | 49.617 | 1.00 15.01 | AAAA |
| ATOM | 1110 | SG | | A 142 | 29.524 | 29.315 | | 1.00 16.45 | AAAA |
| MOTA | 1111 | С | | A 142 | 31.227 | | | 1.00 15.32 | AAAA |
| ATCM | 1112 | 0 | | A 142 | 30.533 | 28.565 | | | AAAA |
| ATOM | 1113 | N | | A 143 | 32.558 | 29.311 | | 1.00 18.63 | AAAA |
| MOTA | 1114 | CA | | A 143 | 33.340 | | | | AAAA |
| ATOM | 1115 | CB | | A 143 | 34.298 | | | | AAAA |
| ATOM | 1116 | CG | TYR | A 143 | 33.664 | | | | AAAA |
| ATOM | 1117 | CD1 | TYR | A 143 | 33.480 | | | | AAAA |
| ATOM | 1118 | CE1 | TYR | A 143 | 32.856 | | | | AAAA |
| ATOM | 1119 | CD2 | TYR | A 143 | 33.212 | | | | AAAA |
| ATOM | 1120 | | TYR | A 143 | 32.588 | | | | AAAA |
| ATOM | 1121 | CZ | | A 143 | 32.414 | | | | AAAA |
| ATCM | 1122 | OH | TYR | A 143 | 31.787 | 33.0/1 | | - • • • • • • • | • |
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|--------------|--------------|----------|---------|-------|---|--------|------------------|---|--------------------------|--------------|
| | 1122 | С | TYR A | 143 | | 34.162 | 27.490 | 46.283 | 1.00 19.06 | AAAA |
| ATOM | 1123 1124 | | TYR A | | | 34.319 | 26.289 | 46.032 | 1.00 18.40 | AAAA |
| ATOM | 1125 | - | ILE A | | | 34.695 | 28.087 | 47.344 | 1.00 19.15 | AAAA |
| MOTA | 1125 | | ILE A | | | 35.490 | 27.350 | 48.315 | 1.00 19.97 | AAAA |
| ATOM | _ | | ILE A | | | 36.952 | 27.861 | 48.355 | 1.00 19.74 | AAAA |
| ATOM | 1127 | | ILE A | | | 37.757 | 27.088 | 49.410 | 1.00 18.03 | AAAA |
| ATOM | 1128 | | ILE A | | | 37.584 | 27.671 | 46.965 | 1.00 20.12 | AAAA |
| MOTA | 1129 | CDI | ILE A | 144 | | 39.053 | 28.072 | 46.846 | 1.00 21.05 | AAAA |
| MOTA | 1130 | | ILE A | | | 34.833 | 27.532 | 49.665 | 1.00 20.22 | AAAA |
| MOTA | 1131 | C . | ILE A | | | 34.357 | 28.626 | 49.981 | 1.00 19.94 | AAAA |
| MOTA | 1132 | | ASN A | | | 34.787 | 26.451 | 50.440 | 1.00 20.57 | AAAA |
| MOTA | 1133 | N | ASN A | | | 34.165 | 26.448 | 51.770 | 1.00 20.39 | AAAA |
| MOTA | 1134 | CA CB | ASN A | | - | 33.450 | 25.114 | 51.990 | 1.00 19.39 | AAAA |
| MOTA | 1135 | CG | ASN A | | | 32.505 | 25.143 | 53.171 | 1.00 19.31 | AAAA |
| MOTA | 1136 | | ASN A | | | 32.862 | 25.583 | 54.263 | 1.00 21.26 | AAAA |
| MOTA | 1137 | ND3 | ASN A | 145 | | 31.290 | 24.667 | 52.960 | 1.00 17.08 | - AAAA |
| ATOM | 1138 | C | ASN A | | | 35.236 | 26.621 | 52.856 | 1.00 20.17 | AAAA |
| MOTA | 1139 | 0 | ASN A | | | 35.690 | 25.622 | 53.421 | 1.00 19.75 | AAAA |
| ATOM | 1140 | N | ASN A | | | 35.644 | 27.862 | 53.148 | 1.00 20.06 | AAAA |
| ATOM | 1141 1142 | CA | ASN A | | | 36.671 | 28.075 | 54.166 | 1.00 20.98 | AAAA |
| ATOM | 1142 | CB | ASN A | | | 37.019 | 29.573 | 54.333 | 1.00 21.78 | AAAA |
| MOTA | | CG | ASN A | | | 35.876 | 30.411 | 54.882 | 1.00 22.78 | AAAA |
| MOTA | 1144 1145 | | ASN A | | | 35.651 | 30.465 | 56.091 | 1.00 22.83 | AAAA |
| MOTA | 1145 | MD2 | ASN A | 146 | | 35.144 | 31.078 | 53.983 | 1.00 23.70 | AAAA |
| MOTA | 1147 | C | ASN A | 146 | | 36.307 | 27.413 | 55.496 | 1.00 21.18 | AAAA |
| ATOM | 1148 | Ö | ASN A | | | 37.169 | 26.823 | 56.139 | 1.00 21.48 | AAAA |
| MOTA | 1149 | N | PRO A | | | 35.031 | 27.476 | 55.922 | 1.00 20.88 | AAAA |
| MOTA | 1150 | CD | PRO A | | | 33.835 | 28.120 | 55.358 | 1.00 21.85 | AAAA |
| ATOM | 1151 | CA | PRO A | | | 34.674 | 26.831 | 57.183 | 1.00 21.42 | AAAA |
| MOTA | 1152 | CB | PRO A | 147 | | 33.176 | 27.073 | 57.261 | 1.00 21.00 | AAAA |
| MOTA MOTA | 1153 | CG | PRO A | | • | 33.052 | 28.408 | 56.605 | 1.00 20.47 | AAAA |
| ATOM | 1154 | c | PRO A | | | 35.015 | 25.334 | 57.174 | 1.00 22.79 | AAAA |
| ATOM | 1155 | Ö | PRO A | | | 35.650 | 24.833 | 58.099 | 1.00 25.69 | AAAA |
| ATOM | 1156 | N | ALA A | | | 34.603 | 24:616 | 56.136 | 1.00 22.34 | AAAA |
| ATOM | 1157 | CA | ALA A | | | 34.889 | 23.193 | 56.070 | 1.00 22.23 | AAAA AAAA |
| MOTA | 1158 | CB | ALA A | | | 34.260 | 22.561 | 54.825 | 1.00 22.87 | AAAA |
| ATOM | 1159 | c | ALA A | | | 36.378 | 22.998 | 56.054 | 1.00 22.33 | AAAA |
| ATOM | 1160 | Ō | ALA A | 148 | | 36.912 | 22.249 | 56.861 | 1.00 23.42 | AAAA |
| ATOM | 1161 | N | VAL A | 149 | | 37.050 | 23.661 | 55.122 | 1.00 22.50 | AAAA |
| ATOM | 1162 | CA | VAL A | 149 | | 38.505 | 23.569 | 55.018 | 1.00 21.29 1.00 20.46 | AAAA |
| ATOM | 1163 | CB | VAL A | | | 39.066 | 24.581 | 54.002 | 1.00 20.40 | AAAA |
| ATOM | 1164 | CG1 | VAL A | 149 | | 40.578 | 24.607 | 54.085 | 1.00 20.03 | AAAA |
| ATOM | 1165 | CG2 | VAL A | A 149 | | 38.608 | 24.229 | 52.593 | 1.00 20.03 | AAAA |
| ATOM | 1166 | С | | A 149 | | 39.164 | 23.848 | 56.367 | 1.00 22.11 | AAAA |
| MOTA | 1167 | 0 | | A 149 | | 40.147 | 23.197 | 56.735 57.088 | 1.00 21.19 | AAAA |
| MOTA | 1168 | N | | A 150 | | 38.628 | 24.826 | 58.386 | 1.00 21.70 | AAAA |
| ATOM | 1169 | CA | GL . | A 150 | | 39.171 | 25.176 | 59.368 | 1.00 22.31 | AAAA |
| MOTA | 1170 | С | | A 150 | | 38.973 | 24.043 | 60.026 | 1.00 22.51 | AAAA |
| ATOM | 1171 | 0 | | A 150 | | 39.913 | 23.597 | 59.453 | 1.00 22.86 | AAAA |
| ATOM | 1172 | N | | A 151 | | 37.736 | 23.566 22.474 | 60.346 | | AAAA |
| MOTA | 1173 | CA | | A 151 | | 37.388 | 22.124 | | 1.00 21.51 | AAAA |
| ATOM | 1174 | CB | | A 151 | | 35.894 | | 61.019 | 1.00 21.36 | AAAA |
| ATOM | 1175 | CG2 | ILE . | A 151 | | 35.542 | 20.899 23.329 | | | AAAA |
| ATOM | 1176 | CGI | L ILE | A 151 | | 35.051 | | | | AAAA |
| ATOM | 1177 | CD1 | L ILE . | A 151 | | 33.576 | 23.199 | | | AAAA |
| MOTA | 1178 | С | ILE | A 151 | | 38.265 | 21.243 | | | AAAA |
| ATOM | 1179 | 0 | | A 151 | | 38.786 | 20.660 | | | AAAA |
| ATCM | 1180 | | | A 152 | | 38.435 | 20.853 | | | AAAA |
| ATOM | 1181 | | | A 152 | | 39.267 | 19.697 | | | AAAA |
| ATOM | 1182 | CB | | A 152 | | 39.242 | 19.404 | | | AAAA |
| ATOM | 1183 | CG | GLU | A 152 | | 37.910 | 18.886 | | | AAAA |
| ATOM | 1184 | CD | | A 152 | | 37.500 | 17.570 | | | AAAA |
| ATOM | 1185 | | 1 GLU | A 152 | | 36.345 | 17.158 | | 05 00 | AAAA |
| ATOM | 1186 | OE: | 2 GLU | A 152 | | 38.315 | | | | AAAA |
| ATOM | 1187 | C | | A 152 | | 40.694 | | | 0/ 40 | AAAA |
| ATOM | | | GLU | A 152 | | 41.425 | 19.035 | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | | • |
| 2.01 | | | • | | | | | | | |

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|--------------|--------------|----------|-------|-------|--------|------------------|------------------|--------------------------|--------------|
| | | | TYR A | 157 | 41.085 | 21.225 | 58.925 | 1.00 27.30 | AAAA |
| ATOM | 1189 | N | TYR A | | 42.422 | 21.632 | 59.334 | 1.00 27.63 | AAAA |
| ATOM | 1190 | CA | TYR A | | 42.532 | 23.153 | 59.268 | 1.00 26.99 | AAAA |
| MOTA | 1191 | CB | TYR A | | 43.856 | 23.719 | 59.710 | 1.00 27.03 | AAAA |
| ATOM | 1192 | CG | | | 44.942 | 23.790 | 58.837 | 1.00 27.78 | AAAA |
| ATOM | 1193 | | TYR A | | 46.165 | 24.356 | 59.250 | 1.00 28.40 | AAAA |
| MOTA | 1194 | | | | 44.017 | 24.215 | 61.007 | 1.00 27.52 | AAAA |
| MOTA | 1195 | | TYR A | | 45.216 | 24.774 | 61.425 | 1.00 27.66 | AAAA |
| ATOM | 1196 | | TYR A | | 46.284 | 24.845 | 60.547 | 1.00 28.15 | AAAA |
| ATOM | 1197 | CZ | TYR A | | 47.457 | 25.407 | 60.974 | 1.00 28.83 | AAAA |
| MOTA | 1198 | OH | TYR A | | 42.618 | 21.172 | 60.769 | 1.00 27.82 | AAAA |
| MOTA | 1199 | C | TYR A | | 43.613 | 20.552 | 61.110 | 1.00 27.15 | AAAA |
| MOTA | 1200 | 0 | TYR A | | 41.636 | 21.487 | 61.604 | 1.00 29.25 | AAAA ` |
| MOTA | 1201 | N | LEU A | | 41.665 | 21.138 | 63.014 | 1.00 29.35 | AAAA |
| MOTA | 1202 | CA | LEU A | | 40.507 | 21.829 | 63.715 | 1.00 30.25 | AAAA |
| MOTA | 1203 | CB | LEU A | 154 | 40.685 | 23.346 | 63.792 | 1.00 31.10 | AAAA |
| MOTA | 1204 | CG | LEU A | | 39.348 | 24.020 | 64.092 | 1.00 31.24 | AAAA |
| MOTA | 1205 | | LEU A | | 41.747 | 23.669 | 64.852 | 1.00 29.84 | AAAA |
| MOTA | 1206 | | LEU A | | 41.625 | 19.639 | 63.263 | 1.00 29.73 | AAAA. |
| MOTA | 1207 | Ç | LEU A | | 42.313 | 19.151 | 64.150 | 1.00 30.51 | AAAA |
| MOTA | 1208 | 0 | ARG A | | 40.832 | 18.903 | 62.489 | 1.00 28.95 | AAAA |
| MOTA | 1209 | N | ARG A | | 40.771 | 17.459 | 62.671 | 1.00 28.94 | AAAA |
| MOTA | 1210 | CA | ARG A | 155 | 39.742 | 16.820 | 61.723 | 1.00 28.64 | AAAA |
| ATOM | 1211 | CB | ARG A | | 38.312 | 17.312 | 61.952 | 1.00 27.82 | AAAA |
| ATOM | 1212 | CG | ARG A | 155 | 37.319 | 16.751 | 60.955 | 1.00 27.19 | AAAA |
| ATOM | 1213 | CD | ARG A | 155 | 36.804 | 15.444 | 61.338 | 1.00 28.86 | AAAA |
| ATOM | 1214 | NE CZ | ARG F | | 35.939 | 14.742 | 60.612 | 1.00 28.93 | AAAA |
| ATOM | 1215 1216 | | ARG A | | 35.500 | 15.227 | 59.459 | 1.00 29.47 | AAAA |
| MOTA | 1217 | MAS | ARG A | 155 | 35.486 | 13.574 | 61.053 | 1.00 28.76 | AAAA |
| MOTA | 1217 | C | ARG A | 155 | 42.158 | 16.853 | 62.438 | 1.00 30.20 | AAAA |
| MOTA | 1219 | ō | | 155 | 42.572 | 15.949 | 63.164 | 1.00 30.74 | AAAA |
| MOTA | 1220 | N | | 156 | 42.890 | 17.362 | 61.447 | 1.00 30.32 | AAAA |
| MOTA | 1221 | CA | LYS | 156 | 44.224 | 16.838 | 61.173 | 1.00 30.07 | AAAA |
| ATOM | 1222 | CB | | 156 | 44.771 | 17.373 | 59.847 | 1.00 30.26 | AAAA |
| MOTA MOTA | 1223 | CG | | A 156 | 46.168 | 16.869 | 59.525 | 1.00 30.16 | AAAA |
| MOTA | 1224 | CD | | A 156 | 46.686 | 17.368 | 58.181 | 1.00 31.19 | AAAA AAAA |
| MOTA | 1225 | CE | | A 156 | 45.884 | 16.813 | 56.986 | 1.00 31.70 | AAAA |
| ATOM | 1226 | NZ | | A 156 | 45.963 | 15.324 | 56.824 | 1.00 31.20 | AAAA |
| MOTA | 1227 | C | | A 156 | 45.167 | 17.202 | 62.306 | 1.00 30.08 1.00 29.16 | AAAA |
| ATOM | 1228 | 0 | LYS A | A 156 | 46.192 | 16.550 | 62.485 | 1.00 29.10 | AAAA |
| ATOM | 1229 | N | LYS | A 157 | 44.816 | 18.252 | 63.053 | 1.00 30.00 | AAAA |
| ATOM | 1230 | CA | LYS | A 157 | 45.608 | 18.691 | 64.196 | 1.00 31.03 | AAAA |
| ATOM | 1231 | CB | | A 157 | 45.446 | 20.201 | 64.452 | 1.00 32.12 | AAAA |
| MOTA | 1232 | CG | LYS . | A 157 | 46.067 | 21.134 | 63.419 | 1.00 32.12 | AAAA |
| ATOM | 1233 | CD | | A 157 | 47.580 | 21.041 | 63.348 62.226 | | AAAF |
| ATOM | 1234 | CE | | A 157 | 48.080 | 21.941 | 61.996 | 1.00 32.74 | AAA |
| ATOM | 1235 | NZ | LYS . | A 157 | 49.556 | 21.921 | 65.458 | 1.00 31.73 | . TAAA |
| MOTA | 1236 | С | | A 157 | 45.196 | 17.923 | 66.558 | 1.00 31.93 | AAAA |
| MOTA | 1237 | 0 | | A 157 | 45.652 | 18.230 | 65.299 | 1.00 32.41 | AAAA |
| MOTA | 1239 | N | | A 158 | 44.312 | 16.942 | | 1.00 32.34 | AAAA |
| MOTA | 1239 | CA | | A 158 | 43.901 | 16.140 | 67.172 | 1.00 32.65 | AAAA |
| ATOM | 1240 | . C | | A 158 | 42.604 | 16.429 | | | AAAA |
| ATOM | 1241 | 0 | | A 158 | 42.182 | 15.604 | | 1.00 33.16 | AAAA |
| ATCM | 1242 | N | | A 159 | 41.960 | 17.565 | | | AAAA |
| ATOM | 1243 | CA | | A 159 | 40.712 | 17.842 19.281 | | | AAAA |
| ATOM | 1244 | CB | | A 159 | 40.220 | | | | AAAA |
| MOTA | 1245 | | | A 159 | 41.134 | 20.343 20.669 | | | AAAA |
| MOTA | 1246 | | 1 PHE | A 159 | 42.327 | 20.009 | | | AAAA |
| MOTA | 1247 | CD: | 2 PHE | A 159 | 40.821 | 21.610 | | | AAAA |
| MOTA | 1248 | | 1 PHE | A 159 | 43.197 | 21.924 | | | AAAA |
| ATOM | 1249 | | | A 159 | 41.689 | | · | | AAAA |
| MOTA | 1250 | | | A 159 | 42.878 | | | | AAAA |
| ATOM | 1251 | | PHE | A 159 | 39.645 | | | | AAAA |
| ATOM | 1252 | | PHE | A 159 | 39.568 | | | | AAAA |
| ATOM | 1253 | | LYS | A 160 | 38.839 | | | | AAAA |
| MOTA | 1254 | CA | LYS | A 160 | 37.794 | 15.415 | , | | |

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|--------------|--------------|-----|-------|-----|-------|---|----------|------------------|------------------|--------------------------|--------------|
| - mos/ | 1255 | СВ | LYS A | Δ. | 160 | | 38.060 | 14.140 | 68.763 | 1.00 33.97 | AAAA |
| MOTA | | | LYS / | | | | | 13.491 | 68.457 | 1.00 35.31 | AAAA |
| MOTA | 1256 1257 | | LYS A | | | | 39.833 | 12.364 | 69.429 | 1.00 36.48 | AAAA |
| MOTA | 1258 | CE | LYS A | Δ . | 160 | | 39.095 | 11.037 | 69.243 | 1.00 37.97 | AAAA |
| ATOM | 1259 | | LYS A | | | | 37.636 | 11.080 | 69.568 | 1.00 39.67 | AAAA |
| MOTA | 1260 | | LYS | | | | 36.385 | 15.941 | 68.210 | 1.00 31.68 | AAAA |
| MOTA | 1261 | | LYS A | | | | 35.405 | 15.290 | 67.887 | 1.00 31.51 | AAAA |
| MOTA | | N | ARG | Δ | 161 | | 36.291 | 17.114 | 68.819 | 1.00 31.11 | AAAA |
| ATOM | 1262 | CA | ARG A | | | | 35.003 | 17.719 | 69.114 | 1.00 30.92 | AAAA |
| MOTA | 1263 | CB | ARG | | | | 34.655 | 17.592 | 70.604 | 1.00 31.78 | AAAA |
| MOTA | 1264 | CG | ARG | | | | 34.451 | 16.157 | 71.102 | 1.00 32.91 | AAAA |
| MOTA | 1265 1266 | CD | ARG | | | | 33.994 | 16.126 | 72.570 | 1.00 33.26 | AAAA |
| MOTA | | NE | ARG | | | | 34.929 | 16.797 | 73.476 | 1.00 34.01 | AAAA |
| MOTA | 1267 | CZ | ARG . | | | | 36.183 | 16.404 | 73.698 | 1.00 34.88 | AAAA |
| MOTA | 1268 1269 | | ARG | | | | 36.675 | 15.334 | 73.081 | 1.00 34.89 | AAAA |
| MOTA | 1270 | MHJ | ARG | Α. | 161 | | 36.954 | 17.084 | 74.537 | 1.00 34.71 | AAAA |
| ATOM | 1271 | C | ARG | | | | 35.061 | 19.185 | 68.714 | 1.00 30.28 | AAAA |
| MOTA | 1271 | Ö | ARG | | | | 35.365 | 20.059 | 69.529 | 1.00 29.86 | AAAA |
| MOTA | 1272 | N | ILE | | | | 34.774 | 19.433 | 67.437 | 1.00 28.86 | AAAA |
| MOTA | 1274 | CA | ILE | | | | 34.788 | 20.774 | 66.862 | 1.00 26.41 | AAAA |
| ATOM | 1275 | CB | ILE | | | | 35.443 | 20.762 | 65.464 | 1.00 26.87 | AAAA |
| MOTA | 1276 | | ILE | | | | 35.453 | 22.160 | 64.872 | 1.00 26.91 | AAAA |
| MOTA | 1277 | | ILE | | | • | 36.877 | 20.234 | 65.578 | 1.00 28.19 | AAAA |
| MOTA | 1277 | | ILE | | | | 37.614 | 20.090 | 64.240 | 1.00 28.24 | AAAA |
| MOTA | 1278 | C | ILE | A | 162 | | 33.369 | 21.283 | 66.731 | 1.00 24.08 | AAAA |
| ATOM ATOM | 1280 | Ö | ILE | | | | 32.485 | 20.572 | 66.267 | 1.00 24.40 | AAAA |
| ATOM | 1281 | N | LEU | | | | 33.153 | 22.519 | 67.153 | 1.00 22.25 | AAAA |
| ATOM | 1282 | CA | LEU | | | | 31.838 | 23.126 | 67.074 | 1.00 20.48 | AAAA |
| ATOM | 1283 | CB | LEU | | | | 31.408 | 23.671 | 68.440 | 1.00 20.97 | AAAA |
| ATOM | 1284 | CG | LEU | | | | 30.099 | 24.477 | 68.486 | 1.00 20.50 | AAAA |
| MOTA | 1285 | | LEU | | | | 28.998 | 23.695 | 67.799 | 1.00 19.07 | AAAA |
| ATOM | 1286 | | LEU | | | | 29.738 | 24.802 | 69.950 | 1.00 19.76 | AAAA |
| MOTA | 1287 | C | LEU | Α | 163 | | 31.801 | 24.241 | 66.055 | 1.00 18.76 | AAAA |
| ATOM | 1288 | ō | LEU | | | | 32.756 | 24.986 | 65.894 | 1.00 18.41 | AAAA |
| MOTA | 1289 | N | | | 164 | | 30.677 | 24.344 | 65.368 | 1.00 17.85 | AAAA AAAA |
| ATOM | 1290 | CA | | | 164 | | 30.496 | 25.372 | 64.373 | 1.00 17.16 | AAAA |
| ATOM | 1291 | CB | TYR | Α | 164 | | 30.644 | 24.768 | 62.983 | 1.00 17.45 | AAAA |
| ATOM | 1292 | CG | TYR | Α | 164 | | 30.484 | 25.783 | 61.900 | 1.00 17.70 | AAAA |
| ATOM | 1293 | CD1 | TYR | Α | 164 | | 31.444 | 26.772 | 61.701 | 1.00 16.23 1.00 17.35 | AAAA |
| ATOM | 1294 | CEl | TYR | Α | 164 | | 31.280 | 27.734 | 60.721 | 1.00 17.95 | AAAA |
| ATOM | 1295 | CD2 | | | 164 | | 29.350 | 25.781 | 61.092 | 1.00 18.03 | AAAA |
| ATOM | 1296 | CE2 | | | 164 | | 29.173 | 26.746 | 60.103 | 1.00 17.30 | AAAA |
| ATOM | 1297 | CZ | | | 164 | | 30.138 | 27.717 | 59.919 58.926 | 1.00 16.70 | AAAA |
| ATOM | 1298 | OH | | | 164 | | 29.955 | 28.647 | 64.514 | 1.00 15.85 | AAAA |
| MOTA | 1299 | С | | | 164 | | 29.123 | 26.016 | 64.416 | 1.00 16.44 | AAAA |
| ATOM | 1300 | 0 | TYR | Α | 164 | | 28.101 | 25.351 | 64.743 | 1.00 15.54 | AAAA |
| ATOM | 1301 | N | ILE | A | 165 | | 29.115 | 27.319 28.088 | 64.897 | 1.00 15.71 | AAAA |
| MOTA | 1302 | | ILE | Α | 165 . | | . 27.878 | 28.819 | 66.250 | 1.00 15.18 | AAAA |
| ATOM | 1303 | CB | | | 165 | | 27.869 | 29.685 | 66.374 | 1.00 13.94 | AAAA |
| MOTA | 1304 | CG2 | ILE | A | 165 | | 26.621 | 27.797 | 67.386 | | AAAA |
| ATOM | 1305 | CG1 | ILE | A | 165 | | 28.000 | 28.421 | 68.747 | | AAAA |
| MOTA | 1306 | | ILE | | | | 28.356 | 29.124 | | 1.00 16.00 | AAAA |
| ATOM | 1307 | C | | | 165 | | 27.808 | 29.941 | 63.576 | | AAAA |
| MOTA | 1308 | 0 | | | 165 | | 28.711 | 29.087 | | | AAAA |
| MOTA | 1309 | N | ASP | A | 166 | | 26.721 | | 61.865 | | AAAA |
| MOTA | 1310 | CA | ASP | A | 166 | | 26.524 | 29.962 29.066 | | | AAAA |
| ATOM | 1311 | СВ | ASP | A | 166 | | 26.240 | 29.809 | | | AAAA |
| ATOM | 1312 | CG | ASP | A | 166 | | 26.238 | 30.659 | | | AAAA |
| ATOM | 1313 | | | | 166 | | 25.353 | | | | AAAA |
| ATOM | 1314 | OD2 | 2 ASP | A | 166 | | 27.131 | 29.521 | | | |
| ATOM | 1315 | С | | | 166 | | 25.342 | 30.904 | | | AAAA |
| MOTA | 1316 | 0 | ASP | Α | 166 | | 24.206 | 30.459 | | | AAAA |
| ATOM | 1317 | | LEU | Α | 167 | | 25.605 | 32.202 | | | AAAA |
| ATOM | 1318 | | LEU | Α | 167 | | 24.526 | 33.135 34.116 | | | аааа |
| ATOM | 1319 | | LEU | A | 167 | | 24.923 | | | | AAAA |
| ATOM | 1320 | CG | LEU | A | 167 | | 25.499 | 33.529 | - | | • |
| | | | | | | | | | | | |

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|--------------|--------------|--------|-----|-----|------------|---|------------------|--------|------------------|------|----------------|--------------|
| ATOM | 1321 | CD1 | LEU | А | 167 | | 25.760 | 34.671 | 65.933 | | 18.72 | AAAA |
| MOTA | 1322 | | LEU | | | | 24.566 | 32.507 | 65.547 | | 17.06 | AAAA |
| ATOM | 1323 | C | LEU | | | | 24.146 | 33.897 | 61.307 | | 17.18 | AAAA |
| ATOM | 1324 | ō | LEU | | | | 23.390 | 34.850 | 61.358 | | 17.21 | AAAA |
| ATOM | 1325 | N | ASP | | | | 24.683 | 33.457 | 60.178 | | 17.83 | AAAA |
| ATOM | 1326 | CA | ASP | | | | 24.382 | 34.067 | 58.904 | | 17.84 | AAAA |
| ATOM | 1327 | | ASP | | | | 25.178 | 33.397 | 57.807 | | 20.42 | AAAA |
| ATOM | 1328 | CG Î | ASP | | | | 25.140 | 34.162 | 56.529 | | 21.41 | AAAA |
| ATOM | 1329 | C | ASP | | | | 22.915 | 33.783 | 58.660 | | 18.35 | AAAA |
| ATOM | 1330 | ō | ASP | | | | 22.419 | 32.722 | 59.032 | | 19.62 | AAAA |
| ATOM | 1331 | | ASP | | | _ | 26.066 | 34.972 | 56.330 | | 22.42 | AAAA |
| ATOM | 1332 | | ASP | | | | 24.186 | 33.971 | 55.746 | | 21.79 | AAAA |
| MOTA | 1333 | N | ALA | | | | 22.239 | 34.717 | 58.010 | | 17.98 | AAAA |
| ATOM | 1334 | CA | ALA | | | | 20.824 | 34.601 | 5 7 .708 | | 17.36 | AAAA |
| MOTA | 1335 | CB | ALA | | | | 20.348 | 35.860 | 57.007 | 1.00 | 17.00 | AAAA |
| ATOM | 1336 | C | ALA | | | | 20.439 | 33.377 | | | 18.64 | AAAA |
| ATOM | 1337 | 0 | | | 169 | | 19.255 | 33.043 | 56.819 | | 19.46 | AAAA |
| ATOM | 1338 | N | | | 170 | | 21.412 | 32.712 | 56.262 | | 18.71 | AAAA |
| ATOM | 1339 | CA | HIS | Α | 170 | | 21.107 | 31.518 | 55.464 | | 18.43 | AAAA |
| ATOM | 1340 | С | HIS | Α | 170 | | 21.802 | 30.265 | 55.986 | | 18.02 | AAAA |
| ATOM | 1341 | 0 | | | 170 | | 22.910 | 30.332 | 56.514 | | 17.20 | AAAA |
| ATOM | 1342 | CB | HIS | Α | 170 | | 21.539 | 31.678 | 54.004 | | 18.79 | AAAA |
| ATOM | 1343 | CG | HIS | Α | 170 | | 21.137 | 32.968 | 53.386 | | 17.65 | AAAA |
| ATOM | 1344 | ND1 | HIS | Α | 170 | | 21.644 | 34.162 | 53.828 | | 18.08 | AAAA |
| ATOM | 1345 | CE1 | HIS | A | 170 | • | 21.112 | 35.081 | 53.054 | | 18.95 | AAAA AAAA |
| MOTA | 1346 | | HIS | | | | 20.301 | 33.194 | 52.348 | | 18.81 | AAAA |
| ATOM | 1347 | NE2 | HIS | | | | 20.291 | 34.544 | 52.140 | | 19.66 17.53 | AAAA |
| ATOM | 1348 | N | | | 171 | | 21.142 | 29.124 | 55.793 | | 16.38 | AAAA |
| ATOM | 1349 | CA | | | 171 | | 21.662 | 27.822 | 56.193 | | 16.32 | AAAA |
| MOTA | 1350 | CB | | | 171 | | 20.644 | 26.740 | 55.830 | | 15.91 | AAAA |
| ATOM | 1351 | CG | | | 171 | | 21.157 | 25.337 | 55.958 55.051 | | 14.14 | AAAA |
| MOTA | 1352 | | | | 171 | | 21.241 | 24.336 | 57.151 | | 16.79 | AAAA |
| MOTA | 1353 | | | | 171 | | 21.602 | 24.807 | 56.973 | 1 00 | 14.91 | AAAA |
| MOTA | 1354 | | | | 171 | | 21.937 | 23.543 | 55.709 | | 15.45 | AAAA |
| MOTA | 1355 | | | | 171 | | 21.725 | 27.522 | 55.509 | | 16.94 | AAAA |
| MOTA | 1356 | C | | | 171 | | 22.982 23.146 | 27.725 | 54.318 | | 18.71 | AAAA |
| MOTA | 1357 | 0 | | | 171 | | 23.140 | 27.019 | 56.279 | | 16.99 | AAAA |
| MOTA | 1358 | N | | | 172 172 | | 25.237 | 26.670 | 55.778 | | 16.23 | AAAA |
| MOTA | 1359 | CA | | | 172 | | 26.219 | 26.721 | 56.947 | | 17.89 | AAAA |
| MOTA | 1360 | CB | | | 172 | | 25.638 | 25.773 | 58.397 | 1.00 | 17.89 | AAAA |
| ATOM | 1361 | SG | | | 172 | | 25.205 | 25.271 | 55.210 | | 16.57 | AAAA |
| ATOM | 1362 1363 | С 0 | CVS | | 172 | | 25.947 | 24.413 | 55.670 | 1.00 | 17.66 | AAAA |
| MOTA | 1364 | N | | | 173 | | 24.364 | 25.026 | 54.214 | 1.00 | 18.25 | AAAA |
| ATOM | 1365 | CA | | | 173 | | 24.253 | 23.680 | 53.620 | 1.00 | 19.91 | AAAA |
| MOTA | 1366 | CB | | | 173 | | 23.342 | 23.699 | 52.397 | 1.00 | 20.86 | AAAA |
| MOTA | 1367 | CG | ASP | Ā | 173 | | 23.780 | 24.719 | 51.358 | 1.00 | 21.90 | AAAA |
| MOTA MOTA | 1368 | | ASP | Ā | 173 | | 23.257 | 24.640 | 50.217 | 1.00 | 21.35 | AAAA |
| ATOM | 1369 | OD2 | ASP | A | 173 | | 24.624 | 25.597 | 51.687 | 1.00 | 21.35 | AAAA |
| ATOM | 1370 | c | | | 173 | | 25.573 | 23.021 | 53.227 | 1.00 | 21.02 | AAAA |
| MOTA | 1371 | ō | ASP | A | 173 | | 25.673 | 21.785 | 53.199 | 1.00 | 22.79 | AAAA |
| ATOM | 1372 | N | GLY | A | 174 | | 26.579 | 23.832 | 52.912 | 1.00 | 20.03 | AAAA |
| ATOM | 1373 | CA | | | 174 | | 27.870 | 23.277 | 52.553 | 1.00 | 19.72 | AAAA |
| ATOM | 1374 | С | | | 174 | | 28.537 | 22.680 | | 1.00 | 20.27 | AAAA |
| ATOM | 1375 | Ō | | | 174 | | 29.110 | 21.599 | 53.711 | 1.00 | 19.77 | AAAA |
| ATOM | 1376 | N | | | 175 | | 28.448 | 23.387 | 54.893 | 1.00 | 21.38 | AAAA |
| ATOM | 1377 | CA | | | 175 | | 29.056 | 22.934 | 56.135 | 1.00 | 22.26 | AAAA |
| ATOM | 1378 | CB | | | 175 | | 29.032 | 24.040 | 57.203 | 1.00 | 23.15 | AAAA AAAA |
| ATOM | 1379 | CG1 | VAL | . ; | 175 | | 29.853 | 23.617 | 58.418 | 1.00 | 22.84 | AAAA |
| ATOM | 1380 | CG2 | VAL | , ; | 175 | | 29.562 | 25.347 | 56.612 | 1.00 | 23.43 | AAAA |
| ATOM | 1381 | C | VAI | , ; | 175 | | 28.302 | 21.724 | 56.654 | 1.00 | 23.51 | AAAA |
| ATOM | 1382 | ŏ | VAI | , 7 | 175 | | 28.893 | 20.803 | 57.210 | 1.00 | 23.74 | AAAA |
| ATOM | 1383 | N | GLN | 1 ; | 176 | | 26.993 | 21.721 | 56.452 | 1.00 | 25.41 | AAAA |
| ATOM | 1384 | CA | GL1 | 1 2 | 176 | | 26.171 | 20.601 | 56.893 | | 24.77 | |
| ATOM | 1385 | CB | GLN | 1 1 | 176 | | 24.689 | | 56.694 | | 26.23 | AAAA |
| ATOM | 1386 | CG | GLN | 1 1 | 176 | | 23.799 | 19.735 | 57.036 | 1.00 | , 20.23 | |
| | | | | | | | | | | | | |

| 3 TOM | 1387 | CD | GLN | Α | 176 | 22.334 | 20.094 | 57.069 | 1.00 27.17 | AAAA |
|-------|------|------|------|-----|-------|--------|----------|----------|------------|--------|
| MOTA | - | | | | | 21.902 | 20.879 | 57.911 | 1.00 28.24 | AAAA |
| ATOM | 1388 | OE1 | | | | | | | | AAAA |
| ATOM | 1389 | NE2 | GLN | A | 176 | 21.556 | 19.522 | 56.151 | 1.00 26.54 | |
| | | | GLN | | | 26.512 | 19.293 | 56.180 | 1.00 25.67 | AAAA |
| MOTA | 1390 | | | | | | | | 1.00 26.98 | AAAA |
| MOTA | 1391 | 0 | GLN- | A | 176 | 26.789 | 18.285 | 56.820 | | |
| | | NT | GLU | 2. | 177 | 26.490 | 19.309 | 54.853 | 1.00 26.34 | AAAA |
| MOTA | 1392 | | | | | _ | | 54.073 | 1.00 26.18 | AAAA |
| MOTA | 1393 | CA | GLU | Α | 177 | 26.786 | 18.117 | | | |
| | | CB | GLU | Δ | 177 | 26.746 | 18.468 | 52.580 | 1.00 27.13 | AAAA |
| MOTA | 1394 | | | | | | 17.269 | 51.628 | 1.00 29.77 | AAAA |
| MOTA | 1395 | | GLU | | | 26.769 | | | 1.00 23.7 | AAAA |
| | 1396 | CD - | GLU | A | 177 | 26.623 | 17.660 | 50.147 | 1.00 31.29 | |
| MOTA | | | | | | 27.655 | 17.935 | 49.500 | 1.00 31.35 | AAAA |
| ATOM | 1397 | OE1 | | | | | | | 1.00 32.05 | AAAA |
| ATOM | 1398 | OE2 | GLU | Α | 177 | 25.471 | 17.703 | 49.636 | | |
| | | | GLU | | | 28.160 | 17.556 | 54.460 | 1.00 26.38 | AAAA |
| ATOM | 1399 | | | | | | | | 1.00 25.41 | AAAA |
| ATOM | 1400 | 0 | GLU | A | 177 | 28.338 | 16.349 | 54.595 | | |
| | | | ALA | | | 29.115 | 18.458 | 54.659 | 1.00 27.58 | AAAA |
| MOTA | 1401 | | | | | | 18.119 | 55.004 | 1.00 27.66 | - AAAA |
| ATOM | 1402 | | ALA | | | 30.495 | | | | AAAA |
| | 1403 | CB | ALA | A · | 178 | 31.345 | 19.385 | 54.994 | 1.00 26.20 | |
| MOTA | | | | | | 30.713 | 17.370 | 56.318 | 1.00 28.33 | AAAA |
| ATOM | 1404 | | ALA | | | | | | 1.00 29.44 | AAAA |
| MOTA | 1405 | 0 | ALA | А | 178 | 31.685 | 16.626 | 56.439 | | |
| | | | PHE | | | 29.849 | 17.564 | 57.308 | 1.00 28.25 | AAAA |
| ATOM | 1406 | N | | | | | 16.852 | 58.561 | 1.00 29.20 | AAAA |
| ATOM | 1407 | CA | PHE | | | 30.036 | | | | AAAA |
| | 1408 | CB | PHE | Α | 179 | 30.570 | 17.794 | 59.624 | 1.00 29.35 | |
| MOTA | | | | | | 31.751 | 18.572 | 59.171 | 1.00 30.26 | AAAA |
| MOTA | 1409 | CG | PHE | | | | | | 1.00 31.01 | AAAA |
| MOTA | 1410 | CD1 | PHE | А | 179 | 31.582 | 19.777 | 58.497 | | |
| | | | | | 179 | 33.033 | 18.069 | 59.339 | 1.00 30.37 | AAAA |
| MOTA | 1411 | | | | | | | 57.993 | 1.00 31.20 | AAAA |
| MOTA | 1412 | CE1 | PHE | Α | 179 | 32.670 | | | 1.00 31.20 | |
| | 1413 | CE2 | PHE | Δ | 179 | 34.133 | 18.749 | 58.840 | 1.00 31.74 | AAAA |
| MOTA | | | | | | | | 58.161 | 1.00 31.81 | AAAA |
| ATOM | 1414 | CZ | PHE | | | 33.950 | | | 1.00 30.33 | AAAA |
| ATOM | 1415 | С | PHE | A | 179 | 28.760 | 16.180 | 59.040 | | |
| | | | | | | 28.624 | 15.810 | 60.215 | 1.00 31.82 | AAAA |
| MOTA | 1416 | , O | PHE | | | | | | 1.00 29.18 | AAAA |
| MOTA | 1417 | N | TYR | Α | 180 | 27.842 | | 58.105 | | |
| | | CA | | | 180 | 26.564 | 15.379 | 58.389 | 1.00 28.99 | AAAA |
| MOTA | 1418 | | | | | 25.725 | | 57.123 | 1.00 28.30 | AAAA |
| ATOM | 1419 | CB | | | 180 | | | | 1.00 28.27 | AAAA |
| MOTA | 1420 | CG | TYR | Α | 180 . | 24.244 | 15.422 | 57.384 | 1.00 28.27 | |
| | | | TYR | | | 23.392 | 14.386 | 57.021 | 1.00 27.05 | AAAA |
| MOTA | 1421 | | | | | | | 57.197 | 1.00 28.51 | AAAA |
| ATOM | 1422 | CE1 | TYR | Α | 180 | 22.029 | | | 1.00 20.32 | AAAA |
| | 1423 | CD2 | TYR | Α | 180 | 23.686 | 16.573 | 57.942 | 1.00 29.34 | |
| MOTA | | | | | | 22.316 | | 58.125 | 1.00 29.27 | AAAA |
| MOTA | 1424 | CE2 | TYR | А | 190 | | | | 1.00 29.33 | AAAA |
| ATOM | 1425 | CZ | TYR | A | 180 | 21.495 | 15.645 | 57.746 | | |
| | | OH | TVD | 2 | 180 | 20.141 | 15.775 | 57.893 | 1.00 30.83 | AAAA |
| MOTA | 1426 | | | | | | | 58.940 | 1.00 28.79 | AAAA |
| ATOM | 1427 | С | | | 180 | 26.673 | | | 1.00 28.71 | AAAA |
| MOTA | 1428 | 0 | TYR | A | 180 | 25.877 | 13.577 | 59.785 | | |
| | | | | | 181 | 27.662 | 13.214 | . 58.472 | 1.00 29.03 | AAAA |
| ATOM | 1429 | N | | | | | | | 1.00 28.49 | AAAA |
| ATOM | 1430 | CA | ASP | A | 181 | 27.813 | | | 1.00 20.49 | · AAAA |
| | 1431 | CB | | | 181 | 28.140 | 10.930 | 57.715 | 1.00 27.59 | |
| MOTA | | | | | | 29.548 | | 57.229 | 1.00 28.82 | AAAA |
| ATOM | 1432 | ÇG | ASP | A | 181 | | | | 1.00 29.25 | AAAA |
| ATOM | 1433 | OD1 | ASP | Α | 181 | 29:981 | . 12 292 | 57.183 | 1.00 29.23 | |
| | | 000 | ASP | | 1 8 1 | 30.216 | | 56.887 | 1.00 28.68 | AAAA |
| ATCM | 1434 | | MOP | A | 101 | | | | 1.00 27.67 | AAAA |
| ATOM | 1435 | С | | | 181 | 28.863 | | | 1 00 27 57 | AAAA |
| | 1436 | ō | | | 181 | 29.271 | . 10.504 | 60.293 | 1.00 27.57 | |
| ATOM | | | LOF | | 101 | 29.308 | 12.713 | | 1.00 26.27 | AAAA |
| ATCM | 1437 | N | | | 182 | | | | 1.00 26.22 | AAAA |
| | 1438 | CA | THR | A | 182 | 30.284 | 12.544 | 61.689 | 1.00 20.22 | |
| ATOM | | | | | | 31.670 | | 61.317 | 1.00 25.92 | AAAA |
| ATOM | 1439 | CB | | | 182 | | | | | AAAA |
| ATCM | 1440 | OG1 | THR | A | . 182 | 32.564 | 12.935 | | 1.00 25.00 | |
| | 1441 | | THR | | | 31.57 | 14.594 | 60.974 | 1.00 25.25 | AAAA |
| MOTA | | | | | | | | | 1.00 25.87 | AAAA |
| ATOM | 1442 | C | | | . 182 | 29.79 | | | | AAAA |
| | 1443 | 0 | THR | ٦ | 182 | 28.942 | 14.102 | | 1.00 20.33 | |
| ATOM | | | | | | 30.32 | | | 1.00 25.86 | AAAA |
| ATCM | 1444 | 11 | | | 183 | | | | | AAAA |
| ATOM | 1445 | CA | ASP | A | 183 | 29.95 | | | | AAAA |
| | 1446 | CB | | | 183 | 29.46 | 3 12.260 | 66.274 | | |
| ATOM | | | | | | 30.51 | | | | AAAA |
| ATCM | 1447 | CG | | | 183 | 30.51 | | | | AAAA |
| | 1448 | נתם | 455 | - 2 | 183 | 31.06 | 3 10.691 | | | |
| ATOM | | | | | | 30.78 | | 67.657 | 1.00 29.21 | ĄAAA |
| ATOM | 1449 | | | | 183 | | | | | AAAA |
| ATCM | 1450 | С | ASP | , | 183 | 31.12 | | | | AAAA |
| | 1451 | 0 | 200 | 2 | 183 | 31.03 | 4 14.566 | | | |
| ATCM | | | | | | 32.22 | | 65.254 | 1.00 26.05 | AAAA |
| ATCM | 1452 | N | GLN | P | 184 | 26.66 | | | | |

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| | | | | _ | , , | | 14 003 | 65.766 | 1.00 25.85 | AAAA |
|-------|------|-----|-----|----------|-----|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 1453 | | GLN | | | 33.381 | 14.983 | 65.095 | 1.00 26.30 | AAAA |
| ATOM | 1454 | | GLN | | | 34.674 | 14.510 | 65.303 | 1.00 27.42 | AAAA |
| ATOM | 1455 | | GLN | | | 34.920 | 13.030 | 64.822 | 1.00 28.40 | AAAA |
| MOTA | 1456 | | GLN | | | 36.273 | 12.583 | 63.709 | 1.00 30.05 | AAAA |
| ATOM | 1457 | OE1 | | | | 36.685 | 12.905 | 65.651 | 1.00 29.24 | AAAA |
| MOTA | 1458 | | GLN | | | 36.970 | 11.816 | | 1.00 25.24 | AAAA |
| MOTA | 1459 | | GLN | | | 33.159 | 16.474 | 65.536 | 1.00 23.22 | AAAA |
| ATOM | 1460 | | GLN | | | 33.734 | 17.316 | 66.220 | 1.00 25.17 | AAAA |
| ATOM | 1461 | N | VAL | Α | 185 | 32.290 | 16.791 | 64.584 | | AAAA |
| ATOM | 1462 | | VAL | | | 31.975 | 18.182 | 64.291 | 1.00 24.49 1.00 23.20 | AAAA |
| ATOM | 1463 | | VAL | | | 32.324 | 18.563 | 62.832 | 1.00 23.20 | AAAA |
| ATOM | 1464 | CG1 | VAL | Α | 185 | 32.045 | 20.060 | 62.599 | 1.00 19.72 | AAAA ' |
| ATOM | 1465 | CG2 | | | | 33.777 | 18.205 | 62.543 | 1.00 20.87 | AAAA |
| ATOM | 1466 | C | VAL | | | 30.494 | 18.421 | 64.501 | 1.00 24.81 | AAAA |
| MOTA | 1467 | 0 | VAL | | | 29.664 | 17.787 | 63.844 | 1.00 27.07 | AAAA |
| ATOM | 1468 | N | PHE | | | 30.162 | 19.311 | 65.434 | 1.00 20.31 | AAAA |
| MOTA | 1469 | CA | | | 186 | 28.768 | 19.645 | 65.684 | 1.00 20.31 | AAAA |
| ATOM | 1470 | CB. | PHE | | | 28.513 | 19.937 | 67.164 | 1.00 13.77 | AAAA |
| MOTA | 1471 | CG | PHE | | | 27.057 | 20.037 | 67.500 | 1.00 13.33 | AAAA |
| ATOM | 1472 | CD1 | PHE | Α | 186 | 26.359 | 18.918 | 67.945 | 1.00 17.70 | AAAA |
| MOTA | 1473 | | PHE | | | 26.358 | 21.213 | 67.263 | 1.00 17.35 | AAAA |
| ATOM | 1474 | | PHE | | | 24.999 | 18.964 | 68.147 | 1.00 17.33 | AAAA |
| ATOM | 1475 | CE2 | PHE | | | 24.997 | 21.271 | 67.459 | 1.00 18.67 | AAAA |
| ATOM | 1476 | CZ | | | 186 | 24.308 | 20.138 | 67.905 | 1.00 18.07 | AAAA |
| ATOM | 1477 | С | | | 186 | 28.464 | 20.911 | 64.895 | 1.00 19.10 | AAAA |
| MOTA | 1478 | 0 | | | 186 | 29.079 | 21.940 | 65.129 | 1.00 18.34 | AAAA |
| MOTA | 1479 | N | | | 187 | 27.520 | 20.834 | 63.964 | 1.00 16.47 | AAAA |
| ATOM | 1480 | CA | | | 187 | 27.137 | 21.993 | 63.160 | 1.00 14.30 | AAAA |
| ATOM | 1481 | CB | | | 187 | 27.006 | 21.630 | 61.655 | 1.00 10.34 | AAAA |
| ATOM | 1482 | | | | 187 | 26.628 | 22.869 | 60.828 | 1.00 10.34 | AAAA |
| ATOM | 1483 | CG2 | | | 187 | 28.314 | 21.031 | 61.160 | 1.00 17.43 | AAAA |
| ATOM | 1484 | С | | | 187 | 25.806 | 22.511 | 63.665 | 1.00 17.45 | AAAA |
| MOTA | 1485 | 0 | VAL | Α | 187 | 24.852 | 21.746 | 63.792 63.960 | 1.00 18.66 | AAAA |
| ATOM | 1486 | N | | | 188 | 25.763 | 23.809 | | 1.00 10.00 | AAAA |
| MOTA | 1487 | CA | | | 188 | 24.555 | 24.507 | 64.460 65.914 | 1.00 21.24 | AAAA |
| MOTA | 1488 | CB | | | 188 | 24.752 | 24.995 | 66.395 | 1.00 20.80 | AAAA |
| MOTA | 1489 | CG | | | 188 | 23.702 | 26.019 | 66.493 | 1.00 19.77 | AAAA |
| ATOM | 1490 | CD1 | LEU | A | 188 | 22.365 | 25.323 26.627 | 67.750 | 1.00 20.63 | AAAA |
| ATOM | 1491 | | | | 188 | 24.085 | 25.735 | 63.591 | 1.00 20.41 | AAAA |
| ATOM | 1492 | С | | | 188 | 24.297 | 26.484 | 63.288 | 1.00 21.86 | AAAA |
| MOTA | 1493 | 0 | | | 188 | 25.223 | 25.987 | 63.233 | 1.00 19.32 | AAAA |
| MOTA | 1494 | N | | | 189 | 23.049 22.786 | 27.130 | 62.381 | 1.00 18.06 | AAAA |
| ATOM | 1495 | CA | | | 189 | | 26.715 | 60.906 | 1.00 18.54 | AAAA |
| MOTA | 1496 | CB | | | 189 | 22.970 | 27.731 | 59.998 | 1.00 17.47 | AAAA |
| MOTA | 1497 | OG | | | 189 | 22.559 | | 62.554 | 1.00 17.90 | AAAA |
| MOT A | 1498 | С | SER | . A | 189 | 21.418 | 27.051 | 62.540 | 1.00 19.54 | AAAA |
| MOLE | 1499 | 0 | SER | . A | 189 | 20.404 21.386 | 29.067 | 62.722 | 1.00 16.97 | AAAA |
| A_OM | 1500 | N | | | 190 | 20.117 | 29.772 | 62.797 | 1.00 18.49 | AAAA |
| MOTA | 1501 | CA | | | 190 | 20.117 | 30.865 | 63.886 | 1.00 17.78 | AAAA |
| ATOM | 1502 | CB | | | 190 | | 30.600 | 65.337 | | AAAA |
| ATOM | 1503 | CG | LEU | A | 190 | 20.534 | 31.406 | 66.266 | 1.00 15.50 | AAAA |
| ATOM | 1504 | CD1 | LEU | A | 190 | | 29.147 | 65.686 | | AAAA |
| MOTA | 1505 | | | | 190 | 20.455 | 30.408 | 61.416 | | AAAA |
| ATOM | 1506 | С | | | 190 | 20.111 | 30.891 | 60.967 | | AAAA |
| MOTA | 1507 | Ō | | | 190 | 21.136 | 30.397 | 60.736 | | AAAA |
| ATOM | 1508 | N | | | 191 | 18.975 | 30.955 | 59.383 | 1.00 23.55 | AAAA |
| MOTA | 1509 | CA | | | 191 | 18.897 | 30.933 | 58.426 | | AAAA |
| ATOM | 1510 | CB | | | 191 | 19.626 | 28.597 | 58.533 | | AAAA |
| ATOM | 1511 | CG | | | 191 | 19.157 | | 59.009 | | AAAA |
| ATOM | 1512 | CD2 | HIS | , A | 191 | 19.770 | 27.485 23.217 | 58.217 | | AAAA |
| MOTA | 1513 | ND1 | HIS | • | 191 | 17.869 | 26.217 | | | AAAA |
| ATOM | 1514 | CE1 | HIS | <i>.</i> | 191 | 17.709 | | | | AAAA |
| MOTA | 1515 | | HIS | , , | 191 | 18.849 | 26.467 31.119 | | | AAAA |
| ATOM | 1516 | | | | 191 | 17.446 | | | | AAAA |
| ATOM | 1517 | | HIS | 5 7 | 191 | 16.519 | 30.658 31.789 | | | АААА |
| ATOM | 1518 | N | GLI | Į | 192 | 17.249 | 31.707 | | | |
| | | | | | | | | | | |

| | | | | | ^ ^6 | 544.0 | | | | |
|--------|------|-----------|-------|----------------|------|---------|------------------|------------------|------------|------|
| MOTA | 1519 | CA | GLN . | A 192 | | 15.899 | 31.959 | 57.269 | 1.00 25.77 | AAAA |
| ATOM | 1520 | CB | GLN | A 192 | | 15.881 | 32.896 | 56.060 | 1.00 26.51 | AAAA |
| ATOM | 1521 | CG | | A 192 | | 16.467 | 34.271 | 56.325 | 1.00 26.99 | AAAA |
| ATOM | 1522 | CD | | A 192 | | 16.581 | 35.076 | 55.062 | 1.00 27.98 | AAAA |
| | 1523 | | | A 192 | | 15.583 | 35.496 | 54.493 | 1.00 30.48 | AAAA |
| ATOM | 1524 | | | A 192 | • | 17.802 | 35.274 | 54.595 | 1.00 29.04 | AAAA |
| ATOM | 1525 | C | | A 192 | | 15.463 | 30.573 | 56.832 | 1.00 25.77 | AAAA |
| | 1526 | ō | | A 192 | | 16.211 | 29.865 | 56.169 | 1.00 26.73 | AAAA |
| - | 1527 | N | | A 193 | | 14.259 | 30.184 | 57.214 | 1.00 25.48 | AAAA |
| MOTA | 1528 | CA | | A 193 | | 13.750 | 28.877 | 56.863 | 1.00 24.51 | AAAA |
| MOTA | 1529 | CB | | A 193 | | 12.288 | 28.788 | 57.286 | 1.00 23.77 | AAAA |
| ATOM | 1530 | OG | | A 193 | | 11.753 | 27.517 | 57.010 | 1.00 24.81 | AAAA |
| ATOM | 1531 | C | | A 193 | | 13.906 | 28.597 | 55.361 | 1.00 24.53 | AAAA |
| MOTA | 1531 | 0 | | A 193 | | 13.736 | 29.479 | 54.522 | 1.00 22.32 | AAAA |
| ATOM | 1533 | N . | | A 194 | | 14.226 | 27.348 | 55.007 | 1.00 25.69 | AAAA |
| ATOM | 1534 | CD | | A 194 | | 14.411 | 26.167 | 55.862 | 1.00 25.02 | AAAA |
| ATOM | 1535 | CA | | A 194 | | 14.399 | 26.976 | 53.604 | 1.00 27.05 | AAAA |
| MOTA | 1536 | CB | PRO | A 194 " | | 14.906 | 25.535 | 53.697 | 1.00 26.30 | AAAA |
| ATOM | 1537 | CG · | | A 194 | | 15.479 | 25.466 | 55.124 | 1.00 26.44 | AAAA |
| ATOM | 1538 | C | | A 194 | | 13.076 | 27.057 | 52.849 | 1.00 27.79 | AAAA |
| ATOM | 1539 | 0 | | A 194 | | 13.066 | 27.057 | 51.625 | 1.00 28.82 | AAAA |
| ATOM | 1540 | N | | A 195 | | 11.966 | 27.133 | 53.582 | 1.00 28.29 | AAAA |
| ATOM | 1541 | CA | | A 195 | | 10.656 | 27.187 | 52.950 | 1.00 29.08 | AAAA |
| MOTA | 1542 | CB | | A 195 | | 9.534 | 27.030 | 54.001 | 1.00 31.08 | AAAA |
| ATOM | 1542 | CG | | A 195 | | 9.070 | 28.294 | 54.722 | 1.00 35.07 | AAAA |
| ATOM | | | | A 195 | | 7.850 | 28.980 | 54 064 | 1.00 38.05 | AAAA |
| ATOM | 1544 | CD OF1 | | A 195 | | 7.389 | 30.017 | 54.601 | 1.00 38.80 | AAAA |
| MOTA | 1545 | OFI | CLU | A 195 | | 7.342 | 28.487 | 53.024 | 1.00 39.20 | AAAA |
| ATOM | 1546 | | | A 195 | | 10.483 | 28.471 | 52.150 | 1.00 28.05 | AAAA |
| MOTA | 1547 | C | | A 195 | | 9.722 | 28.512 | 51.189 | 1.00 28.57 | AAAA |
| MOTA | 1548 | 0 | | A 195 | | 11.223 | 29.510 | 52.514 | 1.00 27.39 | AAAA |
| MOTA | 1549 | N | | | | 11.108 | 30.769 | 51.802 | 1.00 25.80 | AAAA |
| MOTA | 1550 | CA | TYK | A 196 A 196 | | 10.275 | 31.743 | 52.645 | 1.00 24.97 | AAAA |
| MOTA | 1551 | CB | | | | 10.971 | 32.281 | 53.868 | 1.00 23.41 | AAAA |
| MOTA | 1552 | CG | | A 196 | | 11.911 | 33.306 | 53.765 | 1.00 23.99 | AAAA |
| MOTA | 1553 | CD1 | | A 196 | | 12.559 | 33.805 | 54.892 | 1.00 23.44 | AAAA |
| MOTA | 1554 | CE1 | | A 196 | | 10.697 | 31.768 | 55.126 | 1.00 23.24 | AAAA |
| | 1555 | CD2 | TYK | A 196 | | 11.336 | 32.256 | 56.254 | 1.00 23.93 | AAAA |
| MOTA | 1556 | CE2 | | A 196 | | 12.265 | 33.270 | 56.133 | 1.00 24.07 | AAAA |
| MOTA | 1557 | CZ | | A 196 | | 12.913 | 33.731 | 57.247 | 1.00 25.06 | AAAA |
| MOTA | 1558 | OH | TYR | A 196 | | 12.450 | 31.406 | 51.411 | 1.00 24.97 | AAAA |
| ATOM | 1559 | Ċ | TYR | A 196 | | 12.475 | 32.495 | 50.840 | 1.00 25.14 | AAAA |
| ATOM | 1560 | 0 | TYR | A 196 | | 13.563 | 30.737 | 51.686 | 1.00 23.81 | AAAA |
| ATOM | 1561 | N | ALA | A 197 | | 14.855 | 31.330 | 51.337 | 1.00 23.32 | AAAA |
| MOTA | 1562 | CA | | A 197 | | 15.350 | 32.220 | 52.488 | 1.00 23.33 | AAAA |
| ATOM | 1563 | CB | | A 197 | | 15.952 | 30.356 | 50.957 | 1.00 22.74 | AAAA |
| ATOM — | 1564 | C | ALA | A 197 | | 15.951 | 20.330 | .51.37 | 1.00 22.47 | AAAA |
| ATOM | 1565 | | ALA | A 197 | | 16, 900 | 30.852 | 50.16 | 1.00 23.23 | AAAA |
| MOTA | | И | PHE | | | | 30.081 | 49.741 | 1.00 23.68 | AAAA |
| ATOM | 1567 | CA | PHE | A 198 | | 18.062 | | 49.069 | 1.00 23.33 | AAAA |
| MOTA | 1568 | CB | PHE | A 198 | • | 19.083 | 31.006 30.280 | 48.464 | 1.00 22.98 | AAAA |
| MOTA | 1569 | CG | PHE | A 198 | | 20.250 | | 47.203 | 1.00 22.75 | AAAA |
| MOTA | 1570 | CD1 | PHE | A 198 | | 20.151 | 29.713 | 49.175 | 1.00 23.32 | AAAA |
| MOTA | 1571 | CD2 | PHE | A 198 | | 21.436 | 30.127 | | 1.00 22.13 | AAAA |
| ATOM | 1572 | CE1 | PHE | A 198 | | 21.207 | 29.003 | 46.645 48.622 | 1.00 22.83 | AAAA |
| ATOM | 1573 | CE2 | PHE | A 198 | 1 | 22.512 | 29.408 | | 1.00 22.55 | |
| MOTA | 1574 | CZ | | A 198 | , | 22.386 | 28.849 | 47.351 | 1.00 23.69 | AAAA |
| ATOM | 1575 | С | | A 198 | | 18.689 | 29.490 | 51.008 | 1.00 23.09 | AAAA |
| ATOM | 1576 | 0 | PHE | A 198 | | 18.802 | 30.171 | 52.012 | 1.00 23.96 | AAAA |
| ATOM | 1577 | N | PRO | A 199 | | 19.166 | 28.236 | 50.954 | 1.00 24.26 | AAAA |
| MOTA | 1578 | CD | | A 199 | | 19.833 | 27.639 | 52.123 | 1.00 24.20 | AAAA |
| ATOM | 1579 | CA | | A 199 | | 19.199 | 27.286 | | 1.00 23.30 | AAAA |
| ATOM | 1580 | CB | | A 199 | | 20.163 | 26.222 | | 1.00 23.30 | AAAA |
| ATOM | 1581 | CG | | A 199 | | 19.797 | 26.162 | | | AAAA |
| ATOM | 1582 | С | | A 199 | | 17.885 | 26.679 | | | AAAA |
| ATOM | 1583 | 0 | | A 199 | | 17.866 | 26.145 | | | AAAA |
| ATOM | 1584 | N | | A 200 | | 16.811 | 26.756 | 50.116 | 1.00 25.09 | MAMA |
| AION. | | , | | | | | | • | | • |

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| | | | | • | | _ | | 40 763 | 1 00 | 26.29 | AAAA |
|-------|------|------|---------|-------|-------|-----|--------|---------|------|---------|--------|
| ATOM | 1585 | CA . | PHE A | 200 | 15.49 | | | 49.763 | | | AAAA |
| MOTA | 1586 | CB | PHE A | 200 | 15.00 | 54 | | 48.340 | 1.00 | 25.65 | |
| | 1587 | | PHE A | | 14.80 | | | 48.122 | | 24.65 | AAAA |
| ATOM | | CD1 | PHE A | 200 | 15.80 |)6 | 28.781 | 47.439 | | 24.42 | AAAA |
| MOTA | 1588 | CDI | PHE A | 200 | 13.7 | | 28.671 | 48.608 | 1.00 | 23.79 | AAAA |
| MOTA | 1589 | CD2 | PRE A | 200 | 15.6 | | 30.125 | 47.246 | 1.00 | 24.41 | AAAA |
| ATOM_ | 1590 | CEI | PHE A | 200 | 13.5 | | 30.035 | 48.418 | 1.00 | 24.94 | AAAA |
| ATOM | 1591 | CE2 | PHE A | 200 | | | 30.760 | 47.738 | | 24.57 | AAAA. |
| ATOM | 1592 | | PHE A | | 14.4 | | | 49.863 | | 28.54 | AAAA |
| ATOM | 1593 | | PHE A | | 15.4 | | 24.656 | | | 28.76 | AAAA |
| ATOM | 1594 | 0 | PHE A | 200 | 14.3 | | 24.096 | 50.251 | | 29.67 | AAAA |
| ATOM | 1595 | N | GLU A | 201 | 16.4 | 99 | 23.981 | 49.504 | | | |
| | 1596 | | GLU A | | 16.5 | 39 | 22.528 | 49.524 | | 31.88 | AAAA |
| MOTA | 1597 | CB | GLU A | 201 . | 17.4 | 34 | 22.045 | 48.392- | | 32.71 | AAAA |
| ATOM | | | GLU A | | 16.8 | 97 | 22.415 | 47.017 | | 34.87 | AAAA |
| MOTA | 1598 | | GLU A | | 17.8 | | 22.147 | 45.912 | | 35.14 | AAAA |
| ATOM | 1599 | | GLU A | | 18.2 | | 20.982 | 45.735 | | 36.09 | _ AAAA |
| ATOM | 1600 | | | | 18.2 | | 23.112 | 45.221 | 1.00 | 36.30 | AAAA |
| ATOM | 1601 | | GLU A | | 16.9 | | 21.894 | 50.835 | 1.00 | 32.77 | AAAA |
| ATOM | 1602 | _ | GLU A | | | | 20.690 | 51.046 | 1.00 | 33.44 | AAAA |
| MOTA | 1603 | 0 | GLU A | | 16.8 | | | 51.711 | | 32.31 | AAAA |
| ATOM | 1604 | N | LYS A | 202 | 17.5 | | 22.690 | 52.974 | | 32.09 | AAAA |
| ATOM | 1605 | CA | LYS A | 202 | 18.1 | | 22.168 | | 1.00 | 33.02 | AAAA |
| ATOM | 1606 | CB | LYS A | 202 | 19.5 | | 21.750 | 52.811 | 1.00 | 34.95 | AAAA |
| ATOM | 1607 | CG | LYS A | 202 | 19.8 | 36 | 20.847 | 51.623 | 1.00 | 34.33 | AAAA |
| | 1608 | CD | LYS A | 202 | 21.3 | 34 | 20.619 | 51.436 | | 37.92 | |
| MOTA | 1609 | CE | LYS A | 202 | 21.6 | 55 | 19.804 | 50.169 | | 39.19 | AAAA |
| ATOM | _ | NZ | LYS A | 202 | 23.1 | | 19.522 | 49.988 | 1.00 | 38.58 | AAAA |
| MOTA | 1610 | | LYS A | 202 | 17.9 | | 23.241 | 54.037 | | 30.85 | AAAA |
| MOTA | 1611 | C | LYS A | 202 | 17.7 | | 24.389 | 53.739 | | 30.49 | AAAA |
| ATOM | 1612 | 0 | GLY A | 202 . | 18.2 | | 22.867 | 55.281 | 1.00 | 30.81 | AAAA |
| MOTA | 1613 | N | GLY A | 203 | 18.1 | | 23.831 | 56.356 | 1.00 | 30.86 | AAAA |
| ATOM | 1614 | CA | GLY A | 203 | 16.9 | | 23.578 | 57.280 | 1.00 | 30.84 | AAAA |
| MOTA | 1615 | С | GLY A | 203 | 16.8 | | 24.285 | 58.272 | 1.00 | 31.58 | AAAA |
| MOTA | 1616 | 0 | GLY A | 203 | | | 22.570 | 56.965 | | 30.54 | AAAA |
| MOTA | | N | PHE A | 204 | 16.1 | | 22.241 | 57.797 | | 30.51 | AAAA |
| MOTA | 1618 | CA | PHE A | | 15.0 | | 21.317 | 57.058 | | 29.06 | AAAA |
| MOTA | 1619 | CB | PHE A | | 14.0 | | | 55.787 | | 27.13 | AAAA |
| ATOM | 1620 | CG | PHE A | | 13.5 | | 21.890 | 54.601 | 1 00 | 26.52 | AAAA |
| ATOM | 1621 | CD1 | PHE A | 204 | 14. | | 21.762 | | 1.00 | 26.50 | AAAA |
| MOTA | 1622 | CD2 | PHE A | 204 | 12. | | 22.548 | 55.779 | | 26.44 | AAAA |
| ATOM | 1623 | CE1 | PHE A | 204 | 13. | | 22.276 | 53.420 | | 26.69 | AAAA |
| MOTA | 1624 | CE2 | PHE A | 204 | 11. | | 23.069 | 54.600 | | 25.65 | AAAA |
| MOTA | 1625 | CZ | PHE A | 204 | 12. | 190 | 22.931 | 53.416 | 1.00 | 30.87 | AAAA |
| ATOM | 1626 | С | PHE A | 204 | 15.4 | | 21.590 | 59.127 | | | AAAA |
| | 1627 | ō | PHE A | | 16. | 395 | 20.875 | 59.228 | | 31.12 | AAAA |
| MOTA | 1628 | N | LEU A | 205 | 14. | 580 | 21.844 | 60.139 | | 31.22 | AAAA |
| MOTA | 1629 | CA | LEU A | 205 | 14. | | 21.329 | 61.489 | 1.00 | 31.43 | |
| ATOM | | | LEU A | 2.25 | 13. | 575 | 21.691 | 62.357 | 1.00 | 31.42 | AAAA |
| MOTA | 1630 | CB | LEU A | 115 | 13. | | 21.078 | 63.755 | 1.00 | 31.76 | AAAA |
| MOTA | 1631 | CG | LEU A | 235 | 14. | | 21.492 | 64.457 | 1.00 | 32.36 | AAAA |
| ATOM | 1632 | CDI | LEU A | 205 | 12. | | 21.516 | 64.536 | 1.00 | 31.31 | AAAA |
| MOTA | 1633 | | LEU A | 205 | 15. | | 19.829 | 61.625 | 1.00 | 31.35 | AAAA |
| MOTA | 1634 | Č | LEU A | 205 | | | 19.392 | 62.546 | _ | 0 31.40 | AAAA |
| MOTA | 1635 | 0 | LEU A | . 205 | 15. | | 19.059 | 60.707 | 1.0 | 0 31.79 | AAAA |
| ATOM | 1636 | N | GLU A | . 206 | 14. | | | 60.706 | 1 0 | 0 32.08 | AAAA |
| ATOM | 1637 | CA | GLU A | 206 | 14. | | 17.603 | | 1.0 | 0 33.18 | AAAA |
| MOTA | 1638 | CB. | GLU A | . 206 | 13. | | 17.054 | | 1.0 | 0 34.20 | AAAA |
| MOTA | 1639 | CG | GLU A | 206 | 12. | | 17.651 | | | 0 33.44 | AAAA |
| ATOM | 1640 | CD | GLU A | 206 | 11. | | 19.136 | 59.453 | 1.0 | 0 33.32 | AAAA |
| | 1641 | OE1 | GLU A | 206 | 10. | 854 | 19,675 | | | 0 33.32 | AAAA |
| ATOM | 1642 | OF | GLU A | 206 | 13. | 005 | 19:777 | | 1.0 | 0 35.12 | |
| ATOM | | | GLU A | 206 | | 882 | 17.045 | | | 0 32.34 | AAAA |
| MOTA | 1643 | C | GLU A | 206 | | 209 | 15.909 | | | 0 31.83 | AAAA |
| MOTA | 1644 | 0 | GLU A | 200 | | 680 | 17.847 | | | 0 32.48 | AAAA |
| ATOM | 1645 | | GLU A | 207 | | 017 | 17.431 | | 1.0 | 0 31.67 | AAAA |
| MOTA | 1646 | | GLU A | 207 | | 552 | 18.385 | | 1.0 | 0 30.39 | AAAA |
| MOTA | 1647 | | GLU A | 207 | 70. | 768 | | | 1.0 | 0 29.63 | AAAA |
| MOTA | 1648 | CG | GLU A | 20/ | | | 19.547 | 56.121 | | 0 30.04 | AAAA |
| ATOM | 1649 | CD | GLU A | 3 207 | | 953 | 19.991 | 55.971 | 1.0 | 0 30.31 | AAAA |
| ATOM | 1650 | OE: | 1 GLU ? | 1 207 | 19. | 108 | 13.331 | | | | • |
| | | | | • | | | | | | | |

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| | - | | 227 | | 16.947 | 20.070 | 55.604 | 1.00 30.76 | AAAA |
|------|------|------|-------------|---|--------|--------|------------|--------------|--------|
| ATOM | 1651 | OE2 | GLU A 207 | | | 17.433 | 60.537 | 1.00 32.04 | AAAA |
| MOTA | 1652 | C | GLU A 207 | | 18.879 | | 60.910 | 1.00 31.57 | AAAA |
| ATOM | 1653 | 0 | GLU A 207 | | 19.472 | 18.448 | | 1.00 32.57 | AAAA |
| ATOM | 1654 | N | ILE A 208 | • | 18.935 | 16.272 | 61.178 | | AAAA |
| ATOM | 1655 | CA | ILE A 208 | | 19.674 | 16.111 | 62.408 | 1.00 33.37 | |
| | 1656 | CB | ILE A 208 | | 18.709 | 15.647 | 63.519 | 1.00 33.65 | AAAA |
| MOTA | | CD | ILE A 208 | | 19.443 | 15.380 | 64.806 | 1.00 34.11 | AAAA |
| ATOM | 1657 | | | | 17.673 | 16.742 | 63.757 | 1.00 33.94 | · AAAA |
| MOTA | 1658 | | ILE A 208 | | 16.628 | 16.386 | 64.794 | 1.00 37.00 | AAAA |
| MOTA | 1659 | CD1 | ILE A.208 | | | 15.174 | 62.280 | 1.00 34.00 | AAAA |
| ATOM | 1660 | C | ILE A 208 | | 20.863 | | 63.265 | 1.00 34.40 | AAAA |
| ATOM | 1661 | 0 | ILE A 208 | | 21.506 | 14.829 | | 1.00 34.64 | AAAA |
| MOTA | 1662 | N | GLY A 209 | | 21.177 | 14.768 | 61.062 | 1.00 35.55 | AAAA |
| ATOM | 1663 | CA | GLY A 209 | | 22.321 | 13.903 | 60.913 | 1.00 35.55 | AAAA |
| | 1664 | C | GLY A 209 | | 22.164 | 12.671 | 60.057 | 1.00 36.80 | |
| MOTA | | Ö | GLY A 209 | | 21.148 | 12.461 | 59.400 | 1.00 37.32 | AAAA |
| ATOM | 1665 | | GLU A 210 | | 23.199 | 11.836 | 60.100 | 1.00 37.78 | AAAA |
| MOTA | 1666 | N | GLU A 210 | | 23.256 | 10.621 | 59.315 | 1.00 38.04 | AAAA |
| MOTA | 1667 | CA | GLU A 210 | | 23.600 | 11.013 | 57.892 | 1.00 38.54 | AAAA |
| ATOM | 1668 | CB | GLU A 210 | | 23.469 | 9.960 | 56.858 | 1.00 38.99 | AAAA |
| MOTA | 1669 | CG | GLU A 210 | | | 10.412 | 55.580 | 1.00 40.10 | AAAA |
| MOTA | 1670 | CD | GLU A 210 | • | 24.118 | | 55.555 | 1.00 40.86 | AAAA |
| ATOM | 1671 | OE1 | GLU A 210 | | 25.365 | 10.437 | | 1.00 40.41 | AAAA |
| MOTA | 1672 | OE2 | GLU A 210 | | 23.396 | 10.767 | 54.619 | 1.00 37.98 | AAAA |
| ATOM | 1673 | С | GLU A 210 | | 24.377 | 9.770 | 59.894 | | AAAA |
| | 1674 | ŏ | GLU A 210 | | 25.498 | 10.244 | 60.041 | 1.00 38.52 | |
| ATOM | | N | GLY A 211 | | 24.085 | 8.517 | 60.220 | 1.00 38.02 | AAAA |
| ATOM | 1675 | | GLY A 211 | | 25.116 | 7.654 | 60.770 | 1.00 38.09 | AAAA |
| MOTA | 1676 | CA | GLY A 211 | | 25.542 | 8.075 | 62.164 | 1.00 38.26 | AAAA |
| MOTA | 1677 | C | GLI A 211 | | 24.697 | 8.443 | 62.977 | 1.00 37.82 | AAAA |
| MOTA | 1678 | 0 | GLY A 211 | | 26.848 | 8.030 | 62.434 | 1.00 38.20 | AAAA |
| ATOM | 1679 | N | LYS A 212 | | 27.396 | 8.399 | 63.743 | 1.00 37.56 | AAAA |
| MOTA | 1680 | CA | LYS A 212 | | | 8.209 | 63.766 | 1.00 38.86 | AAAA |
| ATOM | 1681 | CB | LYS A 212 | | 28.921 | | 63.385 | 1.00 40.93 | AAAA |
| ATOM | 1682 | CG | LYS A 212 | | 29.416 | 6.810 | | 1.00 42.04 | AAAA |
| ATOM | 1683 | CD | LYS A 212 | | 29.001 | 5.746 | 64.405 | 1.00 42.80 | AAAA |
| ATOM | 1684 | CE | LYS A 212 | | 29.251 | 4.318 | 63.891 | | AAAA |
| | 1685 | NZ | LYS A 212 | | 30.673 | 4.002 | 63.562 | 1.00 42.32 | AAAA |
| ATOM | 1686 | C | LYS A 212 | | 27.093 | 9.859 | 64.054 | 1.00 37.08 | |
| ATOM | | | LYS A 212 | | 27.075 | 10.269 | 65.218 | 1.00 36.94 | AAAA |
| MOTA | 1687 | 0 | GLY A 213 | | 26.854 | 10.636 | 63.002 | 1.00 35.41 | AAAA |
| MOTA | 1688 | N | | | 26.592 | 12.054 | 63.170 | 1.00 34.24 | AAAA |
| MOTA | 1689 | CA | GLY A 213 | | 25.163 | 12.438 | 63.470 | 1.00 33.27 | AAAA |
| ATOM | 1690 | С | GLY A 213 | | 24.861 | 13.611 | 63.666 | 1.00 33.29 | AAAA |
| ATOM | 1691 | 0 | GLY A 213 | | | 11.451 | 63.512 | 1.00 31.79 | AAAA |
| MOTA | 1692 | N | LYS A 214 | | 24.280 | | 63.794 | 1.00 30.47 | AAAA |
| MOTA | 1693 | CA | LYS A 214 | | 22.883 | 11.710 | 63.737 | 1.00 30.35 | AAAA |
| ATOM | 1694 | CB | LYS A 214 | | 22.111 | 10.396 | | 1.00 30.45 | AAAA |
| MOTA | 1695 | CG | LYS A 214 | | 20.676 | 10.552 | 63.280 | 1.00 29.75 | AAAA |
| ATOM | 1696 | | LYS A 214 | | 20.141 | 9.241 | 62.759 | 1.00 29.75 | AAAA |
| | 1697 | | LYS A 214 | | 18.737 | 9.400 | 62.229 | 1.00 30.19 | AAAA |
| MOTA | | | LYS A 214 | | 18.179 | 8.138 | | 1.00 31.35 | |
| MOTA | 1698 | | LYS A 214 | | 22.778 | 12.374 | 65.168 | 1.00 30.31 | AAAA |
| MOTA | 1699 | | LYS A 214 | | 23.193 | 11.814 | | 1.00 30.44 | AAAA |
| ATOM | 1700 | | DIO A 444 | | 22.243 | 13.590 | | 1.00 29.95 | AAAA |
| MOTA | 1701 | | GLY A 215 | | 22.128 | 14.325 | | 1.00 29.16 | AAAA |
| MOTA | 1702 | CA | GLY A 215 | | | 15.379 | | | AAAA |
| ATOM | 1703 | С | GLY A 215 | | 23.222 | | | | AAAA |
| MOTA | 1704 | . 0 | GLY A 215 | | 23.306 | 16.061 | | | AAAA |
| ATOM | 1705 | N | TYR A 216 | | 24.063 | 15.521 | | | AAAA |
| MOTA | 1706 | | | | 25.150 | 16.497 | | | AAAA |
| | 1707 | | | | 26.516 | 15.800 | 65.531 | | AAAA |
| MOTA | 1708 | | | | 26.786 | 14.966 | | | AAAA |
| MOTA | | | 1 TYR A 216 | | 26.138 | | 66.955 | | |
| ATOM | 1709 | | 1 TYR A 216 | | 26.311 | | | 1.00 30.03 | AAAA |
| ATOM | 1710 | | | | 27.619 | | | 1.00 29.71 | AAAA |
| ATOM | 1713 | | 2 TYR A 216 | | | | | 1.00 29.96 | AAAA |
| ATOM | 1712 | | 2 TYR A 216 | | 27.798 | | <u>-</u> - | | AAAA |
| ATOM | | 3 C2 | TYR A 216 |) | 27.143 | | | | AAAA |
| ATCM | | | TYR A 216 | 5 | 27.297 | | | 40 | AAAA |
| MOTA | | | | | 25.055 | | | | AAAA |
| ATOM | | _ | TYR A 216 | | 26.046 | 18.240 | 64.243 | , 1.00 20.50 | • |
| ATOM | | | | | | | | | |
| , | | | | | | | | | |

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| | | | | | 2.2 | 0.45 | 17.791 | 64.076 | 1.00 2 | 23.55 | AAAA |
|-------------|------|-----|-------|-------------|-----|-------|--------|--------|--------|---------|------|
| ATOM | 1717 | N . | ASN A | A 217 | | - | | 63.119 | 1.00 2 | 1 52 | AAAA |
| ATOM | 1718 | CA | ASN A | A 217 | | | 18.830 | | | | AAAA |
| | _ | | | A 217 | 23. | | 18.282 | 61.699 | 1.00 2 | | |
| MOTA | 1719 | | | A 217 | | 202 | 19.386 | 60.669 | 1.00 2 | | AAAA |
| MOTA | 1720 | | | | | 089 | 19.888 | 60.499 | 1.00 | 18.03 | AAAA |
| ATOM | 1721 | OD1 | ASN 7 | A 217 | | | | 60.004 | 1.00 | 19 95 | AAAA |
| ATOM | 1722 | ND2 | ASN A | A 217 | | 274 | 19.790 | | 1.00 | 11 64 | AAAA |
| | 1723 | C | NZA | A 217 | 22. | 216 | 19.346 | 63.605 | 1.00 | 21.04 | |
| MOTA | | | | A 217 | | 263 | 18.576 | 63.757 | 1.00 | 20.34 | AAAA |
| ATOM | 1724 | 0 | ASN . | A 217 | | 165 | 20.647 | 63.873 | 1.00 | 22.22 | AAAA |
| ATOM | 1725 | N | LEU . | A 218 | | | | 64.388 | 1.00 | 22.03 | AAAA |
| ATOM | 1726 | CA | LEU . | A 218 | | .960 | 21.282 | | 1.00 | 20 97 | AAAA |
| | 1727 | CB | LEU | A 218 | 21 | . 195 | 21.711 | 65.840 | 1.00 | 20.37 | AAAA |
| MOTA | | | | A 218 | 20 | .051 | 21.838 | 66.841 | 1.00 | 20.94 | |
| MOTA | 1728 | CG | - EU | 210 | | .513 | 22.744 | 67.936 | 1.00 | 20.31 | AAAA |
| ATOM | 1729 | CDI | LEU | A 218 | | | 22.412 | 66.227 | 1.00 | 21.27 | AAAA |
| ATOM | 1730 | CD2 | LEU | A 218 | | .818 | | 63.547 | 1.00 | 22.70 | AAAA |
| ATOM | 1731 | С | LEU | A 218 | | . 669 | 22.513 | 63.547 | 1.00 | 22 64 | AAAA |
| | 1732 | ō | LEU. | A 218 | 21 | .451 | 23.454 | 63.557 | 1.00 | 22.04 | |
| MOTA | | | D CNI | A 219 | 19 | .564 | 22.491 | 62.808 | 1.00 | 24.00 | AAAA |
| MOTA | 1733 | N | ASN | 210 | | .166 | 23.626 | 61.990 | 1.00 | 25.33 | AAAA |
| ATOM | 1734 | CA | ASN | A 219 | | | 23.190 | 60.614 | 1.00 | 26.94 | AAAA |
| ATOM | 1735 | CB | ASN | A 219 | | .656 | | 59.749 | 1 00 | 26.68 | AAAA |
| | 1736 | CG | ASN | A 219 | 19 | .737 | 22.601 | | 1.00 | 20.00 | AAAA |
| ATOM | | 001 | ΔSM | A 219 | 20 | .812 | 23.169 | 59.626 | 1.00 | 28.06 | |
| ATOM | 1737 | 001 | N CN | A 219 | | .446 | 21.471 | 59.117 | 1.00 | 26.26 | AAAA |
| ATOM | 1738 | | ASN | A 219 | | .046 | 24.345 | 62.710 | 1.00 | 25.69 | AAAA |
| ATOM | 1739 | C | ASN | A 219 | | | | 63.210 | 1 00 | 27.51 | AAAA |
| ATOM | 1740 | 0 | ASN | A 219 | | .118 | 23.706 | | 1 00 | 25.05 | AAAA |
| | 1741 | N | ILE | A 220 | 18 | .122 | 25.667 | 62.753 | | | AAAA |
| MOTA | | CA | TÌE | A 220 | 17 | .107 | 26.457 | 63.428 | | 25.87 | |
| MOTA | 1742 | | T T E | A 220 | | .733 | 27.331 | 64.557 | 1.00 | 25.04 | AAAA |
| MOTA | 1743 | CB | ڪيا ن | A 220 | | .654 | 28.152 | 65.227 | 1.00 | 25.24 | AAAA |
| ATOM | 1744 | CG2 | ILE | A 220 | | | 26.447 | 65.584 | 1.00 | 24.07 | AAAA |
| MOTA | 1745 | CG1 | ILE | A 220 | | .460 | | | 1 00 | 22.28 | AAAA |
| | 1746 | CD1 | ILE | A 220 | | .557 | 25.502 | 66.378 | 1.00 | 26.20 | AAAA |
| MOTA | | C | TLE | A 220 | 16 | .430 | 27.370 | 62.414 | 1.00 | 26.20 | |
| MOTA | 1747 | | TIE | A 220 | | .801 | 28.534 | 62.265 | 1.00 | 25.35 | AAAA |
| MOTA | 1748 | 0 | 115 | A 220 | | .421 | 26.850 | 61.704 | 1.00 | 26.70 | AAAA |
| MOTA | 1749 | N | PRO | A 221 | | | 25.501 | 61.778 | 1.00 | 27.17 | AAAA |
| ATOM | 1750 | CD | | A 221 | | .840 | | | 1 00 | 27.67 | AAAA |
| ATOM | 1751 | CA | PRO | A 221 | 14 | .706 | 27.640 | 60.703 | 1.00 | 26.81 | AAAA |
| | _ | CB | | A 221 | 13 | .771 | 26.613 | 60.064 | 1.00 | 20.01 | |
| ATOM | 1752 | | DBO | A 221 | | .473 | 25.293 | 60.346 | 1.00 | 27.36 | AAAA |
| MOTA | 1753 | CG | PRO | 221 | | .944 | 28.763 | 61.390 | | 28.61 | AAAA |
| MOTA | 1754 | C | PRO | A 221 | | | 28.515 | 62.363 | 1.00 | 29.91 | AAAA |
| MOTA | 1755 | 0 | PRO | A 221 | | 3.218 | | | 1 00 | 28.15 | AAAA |
| MOTA | 1756 | N | LEU | A 222 | | 1.100 | 29.990 | 60.900 | 1.00 | 28.48 | AAAA |
| | 1757 | CA | L.E.U | A 222 | 13 | 3.408 | 31:117 | 61.511 | 1.00 | 20.40 | AAAA |
| MOTA | | | 1 511 | A 222 | | 1.431 | 32.041 | 62.191 | 1.00 | 28.69 | |
| MOTA | 1758 | CB | | 2 222 | | 5.187 | 31.394 | 63.371 | 1.00 | 28.67 | AAAA |
| MOTA | 1759 | CG | LEU | A 222 | | | 32.300 | 63.837 | 1.00 | 28.62 | AAAA |
| MOTA | 1760 | CD1 | LEU | A 222 | 1.0 | 5.304 | | 64.527 | 1 00 | 27.65 | AAAA |
| ATOM | 1761 | CD2 | LEU | A 222 | 14 | 4.231 | 31.106 | | | 28.44 | AAAA |
| | 1762 | C | | A 222 | 1. | 2 26 | 31.882 | 60.518 | 1.00 | 20.44 | AAAA |
| ATOM | | | t EII | A 222 | | 2.318 | 31.958 | 59.325 | 1.00 | 27.90 | |
| MOTA | 1763 | 0 | 220 | A 223 | | 113 | 32.441 | 61.009 | 1.00 | 28.79 | AAAA |
| MOTA | 1764 | N | PRO | - 223 | | 0.966 | 32.357 | 62.410 | 1.00 | 29.20 | AAAA |
| ATOM | 1765 | CD | PRO | A 223 | | | | 60.227 | 1.00 | 29.36 | AAAA |
| MOTA | 1766 | CA | PRO | A 223 | | 0.437 | 33.202 | | | 28.98 | AAAA |
| | 1767 | CB | PRO | A 223 | | 9.256 | 33.287 | | | 20.50 | AAAA |
| MOTA | | | DPA | A 223 | | 9.965 | 33.502 | 62.485 | | 28.68 | |
| MOTA | 1768 | | PRO | , , , , , , | | 0.890 | 34.585 | | 1.00 | 30.15 | AAAA |
| MOTA | 1769 | С | PRO | A 223 | | | 35.152 | | | 30.18 | AAAA |
| ATOM | 1770 | 0 | PRC | A 223 | | 1.864 | | | | 30.50 | AAAA |
| ATOM | 1771 | N | LYS | A 224 | | 0.150 | 35.112 | | | 29.92 | |
| | 1772 | | T.YS | A 224 | 1 | 0.398 | 36.422 | 58.213 | | 20.52 | AAAA |
| ATOM | | | tve | A 224 | | 9.491 | 36.661 | 57.008 | | 30.57 | |
| MOTA | 1773 | | 1112 | , , , , , , | | 9.588 | 35.676 | | 1.00 | 30.06 | AAAA |
| MOTA | 1774 | | LYS | A 224 | | | | | 1.00 | 30.91 | AAAA |
| MOTA | 1775 | CD | LYS | A 224 | | 8.640 | | | | 32.15 | AAAA |
| ATOM | 1776 | | LYS | S A 224 | | 8.575 | | | | 32.75 | AAAA |
| | | | 7.79 | A 224 | | 7.628 | 35.476 | | | 0 20 75 | AAAA |
| MOTA | | | 7 77 | A 224 | 1 | 0.050 | | 59.260 | | 0 29.75 | |
| MOTA | | | LI | | - | 9.308 | | | 1.0 | 0 29.84 | AAAA |
| ATOM | | | LYS | 5 A 224 | _ | | | | 1.0 | 0 29.39 | АААА |
| ATOM | |) N | GL: | Y A 225 | | 0.555 | | | | 0 29.87 | AAAA |
| ATOM | | | GL: | Y A 225 | | 0.261 | | | | 0 29.85 | AAAA |
| MOTA | | | GL' | Y A 225 | 1 | 0.809 | 39.447 | 61.41 | J 1.0 | | • |
| - A I I M*I | | | | | | | | | | | |

| | | _ | CT 1/ | x | 225 | | 10.371 | 40.051 | 62.392 | 1.00 29.85 | AAAA |
|--------------|--------------|----------|----------------|---------------|------------|---|------------------|------------------|------------------|--------------------------|--------------|
| ATOM | 1783 | | GLY . LEU . | | | | 11.775 | 38.536 | 61.499 | 1.00 29.50 | AAAA |
| ATOM | 1784 | N | LEU . | γ. | 226 | | 12.374 | 38.175 | 62.778 | 1.00 29.80 | AAAA |
| ATOM | 1785 | CA | LEU . | ν | 226 | | 13.513 | 37.170 | 62.570 | 1.00 28.81 | AAAA |
| MOTA | 1786 | | LEU | | | | 14.097 | 36.514 | 63.820 | 1.00 27.29 | AAAA |
| MOTA | 1787 | | LEU . | | | | 13.132 | 35.452 | 64.275 | 1.00 26.06 | AAAA |
| ATOM | 1788 | CDI | LEU . | ν | 226 | | 15.455 | 35.888 | 63.538 | 1.00 27.03 | AAAA |
| MOTA | 1789. | | LEU | | | | 12.936 | 39.428 | 63.448 | 1.00 30.68 | AAAA |
| MOTA | 1790 | | LEU | | | | 13.636 | 40:217 | 62.804 | 1.00 30.57 | AAAA |
| MOTA | 1791 | | ASN | Δ | 227 | | 12.624 | 39.617 | 64.729 | 1.00 31.46 | AAAA |
| MOTA | 1792 1793 | N CA | ASN | | | | 13.139 | 40.769 | 65.469 | 1.00 32.06 | AAAA |
| MOTA | | CB | ASN | | | • | 12.012 | 41.507 | 66.217 | 1.00 31.74 | AAAA |
| MOTA | 1794 1795 | CG | ASN | | | | 11.291 | 40.630 | 67.234 | 1.00 32.07 | AAAA |
| ATOM | 1796 | | ASN | | | | 11.914 | 40.017 | 68.104 | 1.00 31.61 | AAAA |
| MOTA | 1797 | ND2 | ASN | A | 227 | | 9.962 | 40.592 | 67.141 | 1.00 31.59 | AAAA |
| MOTA | 1798 | C | ASN | Α | 227 | | 14.225 | 40.334 | 66.444- | 1.00 32.45 | AAAA |
| MOTA | 1799 | Õ | ASN | | | | 14.413 | 39.140 | 66.688 | 1.00 32.78 | AAAA |
| ATOM ATOM | 1800 | N | ASP | | | · | 14.943 | 41.297 | 67.002 | 1.00 33.32 | AAAA |
| ATOM | 1801 | CA | ASP | | | | 16.017 | 40.976 | 67.928 | 1.00 34.75 | AAAA |
| ATOM | 1802 | CB | ASP | | | | 16.508 | 42.233 | 68.654 | 1.00 36.77 | AAAA AAAA |
| ATOM | 1803 | CG | ASP | | | | 17.154 | 43.238 | 67.714 | 1.00 37.28 | AAAA |
| MOTA | 1804 | OD1 | ASP | Α | 228 | | 17.662 | 42.816 | 66.652 | 1.00 37.78 | AAAA |
| ATOM | 1805 | OD2 | ASP | Α | 228 | | 17.180 | 44.443 | 68.054 | 1.00 37.21 | AAAA |
| ATOM | 1806 | С | ASP | Α | 228 | | 15.707 | 39.892 | 68.964 | 1.00 34.93 1.00 36.92 | AAAA |
| ATOM | 1807 | 0 | ASP | | | | 16.448 | 38.919 | 69.056 | 1.00 38.92 | AAAA |
| ATOM | 1808 | N | ASN | | | | 14.635 | 40.054 | 69.741 | 1.00 33.90 | AAAA |
| ATOM | 1809 | CA | ASN | Α | 229 | | 14.268 | 39.079 | 70.775 | 1.00 33.01 | AAAA |
| ATOM | 1810 | CB | ASN | | | | 12.965 | 39.481 | 71.455 72.369 | 1.00 34.04 | AAAA |
| ATOM | 1811 | CG | ASN | | | | 13.131 | 40.663 | 73.405 | 1.00 34.25 | AAAA |
| ATOM - | 1812 | OD1 | ASN | A | 229 | | 13.783 | 40.564 41.797 | 71.988 | 1.00 34.05 | AAAA |
| MOTA | 1813 | | ASN | A | 229 | | 12.550 | 37.656 | 70.276 | 1.00 32.98 | AAAA |
| MOTA | 1814 | С | ASN | A | 229 | | 14.114 14.529 | 36.697 | 70.944 | 1.00 32.77 | AAAA |
| MOTA | 1815 | 0 | ASN | | | | 13.496 | 37.523 | 69.108 | 1.00 32.02 | AAAA |
| ATOM | 1816 | N | | | 230 | | 13.277 | 36.227 | 68.516 | 1.00 30.72 | AAAA |
| MOTA | 1817 | CA | | | 230 230 | | 12.399 | 36.375 | 67.272 | 1.00 31.38 | AAAA |
| ATOM | 1818 | CB | | | 230 | | 11.006 | 36.896 | 67.583 | 1.00 31.02 | AAAA |
| ATOM | 1819 | CG CD | | | 230 | | 10.175 | 37.187 | 66.350 | 1.00 31.52 | AAAA |
| MOTA | 1820 1821 | | GLU | | | | 10.644 | 37.970 | 65.497 | 1.00 31.89 | AAAA |
| MOTA | 1822 | | GLU | | | | 9.047 | 36.655 | 66.241 | 1.00 31.04 | AAAA |
| ATOM | 1823 | C | GLU | A | 230 | | 14.628 | 35.622 | 68.180 | 1.00 30.79 | AAAA |
| ATOM ATOM | 1824 | õ | GLU | A | 230 | | 14.905 | 34.465 | 68.512 | 1.00 31.05 | AAAA |
| ATOM | 1825 | N | PHE | A | 231 | • | 15.490 | 36.412 | 67.553 | 1.00 30.05 | AAAA AAAA |
| MOTA | 1826 | CA | | | 231 | | 16.811 | 35.920 | 67.191 | 1.00 28.94 | AAAA |
| ATOM | 1827 | CB | PHE | Α | 231 | | 17.632 | 37.015 | 66.528 | 1.00 29.33 | AAAA |
| ATOM | 1828 | CĠ | PHE | Α | 231 | | 18.949 | 36.537 | 65.972 | 1.00 28.79 1.00 28.93 | AAAA |
| MOTA | 1829 | CD1 | PHE | Α | 231 | | 18.982 | 35.585 | 64.957 | 1.00 28.55 | AAAA |
| ATOM | 1830 | CD2 | PHE | A | 231 | | 20.152 | 37.067 | 66.436 | 1.00 28.32 | AAAA |
| MOTA | 1831 | CE1 | PHE | A | 231 | | 20.195 | 35.160 | 64.397 65.888 | 1.00 28.97 | AAAA |
| ATOM | 1832 | CE2 | PHE | A | 231 | | 21.376 | 36.657 | 64.860 | | AAAA |
| MOTA | 1833 | CZ | | | 231 | | 21.397 | 35.695 | 68.413 | 1.00 28.25 | AAAA |
| ATOM | 1834 | С | PHE | A | . 231 | | 17.559 | | 68.485 | | AAAA |
| MOTA | 1835 | 0 | PHE | A | 231 | | 17.999 | 36.329 | 69.384 | | AAAA |
| ATOM | 1836 | N | | | 232 | | 17.691 | | 70.590 | | AAAA |
| ATOM | 1837 | CA | | | 232 | | 18.425 | | 71.484 | 1.00 28.16 | AAAA |
| MOTA | 1838 | CB | | | 232 | | 18.521 19.220 | | 70.747 | | AAAA |
| MOTA | 1839 | CG | LEU | A | 232 | | 19.220 | | 71.587 | | AAAA |
| ATOM | 1840 | CDI | LEU | , A | 232 | | 20.639 | | | | AAAA |
| ATOM | 1841 | | LEU | <u>ج</u> - | 232 | | 17.815 | | | | AAAA |
| ATOM | 1842 | C | ĿΕU | ڊر د | 232 | | 18.526 | | | 1.00 27.92 | AAAA |
| ATOM | 1843 | | LEU | تر ج | 232 233 | | 16.495 | | | 1.00 28.81 | AAAA |
| ATCM | 1844 | | PHE | نو • | 233 | | 15.786 | | | 1.00 30.27 | AAAA |
| ATOM | 1845 | | PHE | , , | 233 | | 14.278 | | | 1.00 31.51 | AAAA |
| ATOM | 1846 | | | | 233 | | 13.465 | | | 1.00 32.38 | AAAA |
| ATOM | 1847 | | rnt Put | , , | A 233 | | 13.257 | | | | AAAA |
| ATOM | 1948 | CD. | · Luc | | . 233 | | | | • | | • |

| | 1040 | CD2 | PHE A | 233 | 12.928 | 31.741 | 71.467 | 1.00 33.51 | AAAA |
|--------|------|-----|---------|-------------------|--------|--------------|---------|------------|--------|
| MOTA | 1849 | | PHE A | 233 | 12.518 | 31.537 | 74.201 | 1.00 35.10 | AAAA |
| ATOM | 1850 | | | | 12.193 | 30.677 | 71.975 | 1.00 34.21 | AAAA |
| ATOM | 1851 | | PHE A | | 11.986 | 30.572 | 73.344 | 1.00 35.23 | AAAA |
| ATOM | 1852 | CZ | PHE A | | | 32.301 | 71.483 | 1.00 30.55 | AAAA |
| ATOM | 1853 | С | PHE A | | 16.219 | | 72.280 | 1.00 30.65 | AAAA |
| ATOM - | 1854 | 0 | PHE A | 233 | 16.438 | 31.391 | | 1.00 30.21 | AAAA |
| ATOM | 1855 | N | ALA A | 234 | 16.317 | 32.151 | 70.165 | | AAAA |
| | 1856 | CA | ALA A | 234 | 16.698 | 30.892 | 69.549 | 1.00 28.97 | |
| MOTA | 1857 | СВ | ALA A | | 16.398 | 30.942 | 68.065 | 1.00 30.40 | AAAA |
| MOTA | | C | ALA A | | 18.169 | 30.571 | 69.761 | 1.00 28.27 | AAAA |
| MOTA | 1858 | | ALA A | | 18.564 | 29.401 | 69.830 | 1.00 26.69 | AAAA |
| MOTA | 1859 | 0 | LEU ? | 2 225 | 18.978 | 31.614 | 69.855 | 1.00 27.56 | AAAA |
| MOTA | 1860 | N | LEU A | 1,233 | 20.402 | 31.427 | 70.055- | 1.00 29.17 | AAAA |
| MOTA | 1861 | CA | LEU A | | 21.126 | 32.767 | 69.989 | 1.00 29.04 | AAAA |
| ATOM | 1862 | CB | LEU A | 1 235 | | 32.757 | 69.378 | 1.00 28.54 | AAAA |
| ATOM | 1863 | CG | LEU A | | 22.527 | | 70.058 | 1.00 27.05 | - AAAA |
| MOTA | 1864 | CD1 | LEU A | A 235 | 23.350 | 33.837 | 69.558 | 1.00 27.21 | AAAA |
| ATOM | 1865 | CD2 | LEU A | A 235 | 23.182 | 31.408 | | 1.00 30.99 | AAAA |
| ATOM | 1866 | С | LEU 2 | A 235 | 20.637 | 30.799 | 71.429 | 1.00 30.55 | AAAA |
| MOTA | 1867 | 0 | LEU A | A 235 | 21.159 | 29.697 | 71.547 | | AAAA |
| | 1868 | N | | A 236 | 20.242 | 31.514 | 72.471 | 1.00 31.88 | AAAA |
| MOTA | 1869 | CA | | A 236 | 20.409 | 31.042 | 73.838 | 1.00 32.99 | |
| ATOM | | CB | | A 236 | 19.689 | 31.990 | 74.790 | 1.00 34.63 | AAAA |
| MOTA | 1870 | | | A 236 | 19.980 | 33.449 | 74.531 | 1.00 36.79 | AAAA |
| ATOM | 1871 | CG | | A 236 | 19.044 | 34.360 | 75.294 | 1.00 38.99 | AAAA |
| MOTA | 1872 | CD | GLU A | A 230 | 17.803 | 34.303 | 75.070 | 1.00 39.03 | AAAA |
| ATOM | 1873 | OE1 | GLU . | A 230 | 19.559 | 35.132 | 76.126 | 1.00 41.56 | AAAA |
| ATOM | 1874 | | GLU . | A 236 | 19.806 | 29.656 | 73.982 | 1.00 32.94 | AAAA |
| MOTA | 1875 | С | | A 236 | | 28.753 | 74.595 | 1.00 31.76 | AAAA |
| ATOM | 1876 | 0 | GLU . | A 236 | 20.379 | | 73.399 | 1.00 32.83 | AAAA |
| MOTA | 1877 | Ŋ | LYS | A 237 | 18.631 | 29.503 | 73.471 | 1.00 33.59 | AAAA |
| ATOM | 1878 | CA | LYS | A 237 | 17.906 | 28.256 | | 1.00 35.00 | AAAA |
| MOTA | 1879 | CB | LYS | A 237 | 16.504 | 28.506 | 72.942 | 1.00 35.60 | AAAA |
| ATOM | 1880 | ĊĠ | LYS | A 237 | 15.516 | 27.436 | 73.213 | 1.00 30.09 | AAAA |
| | 1881 | CD | LYS | A 237 | 14.310 | 28.008 | 73.940 | 1.00 38.53 | AAAA |
| MOTA | 1882 | CE | LYS | A 237 | 14.636 | 28.331 | 75.392 | 1.00 39.27 | |
| ATOM | | NZ | LVS | A 237 | 13.398 | 28.531 | 76.204 | 1.00 39.42 | AAAA |
| MOTA | 1883 | | TVC | A 237 | 18.619 | 27.129 | 72.707 | 1.00 33.14 | AAAA |
| ATOM | 1884 | C | TVC. | A 237 | 18.850 | 26.051 | 73.260 | 1.00 33.29 | AAAA |
| MOTA | 1885 | 0 | | A 238 | 18.985 | 27.374 | 71.452 | 1.00 32.13 | AAAA |
| MOTA | 1886 | N | SER | M 230 | 19.671 | 26.345 | 70.685 | 1.00 31.25 | AAAA |
| MOTA | 1887 | CA | SER | A 238 | 19.740 | 26.717 | 69.194 | 1.00 30.52 | AAAA |
| MOTA | 1888 | CB | SER | A 238 | 20.544 | 27.851 | 68.970 | 1.00 29.95 | AAAA |
| MOTA | 1889 | OG | SER | A 238 | | 26.064 | 71.236 | 1.00 31.21 | AAAA |
| MOTA | 1890 | С | SER | A 238 | 21.075 | 24.929 | 71.169 | 1.00 30.06 | AAAA |
| MOTA | 1891 | . 0 | SER | A 238 | 21.556 | - | 71.782 | 1.00 31.71 | AAAA |
| MOTA | 1892 | N | LEU | A 239 | 21.740 | | 72.351 | 1.00 33.47 | AAAA |
| ATOM | 1893 | CA | LEU | A 239 | 23.070 | | 72.331 | 1.00 31.25 | AAAA |
| ATOM | 1894 | CB | LEU | A 239 | 23.698 | | | 1.00 29.80 | AAAA |
| ATOM | 1895 | CG | LEU | A 239 | 23.988 | | 71.977 | 1.00 29.00 | AAAA |
| MOTA | 1896 | CDI | LEU | A 239 | 24.589 | | 72.787 | 1.00 29.05 | AAAA |
| | 1897 | CD | LEU | A 239 | 24.919 | 28.903 | 70.872 | 1.00 29.36 | |
| MOTA | 1898 | c | UEU | A 239 | 22.933 | 25.839 | | 1.00 35.41 | AAAA |
| MOTA | | ō | TEII | A 239 | 23.812 | | 73.735 | 1.00 36.25 | AAAA |
| MOTA | 1899 | | | A 240 | 21.816 | | | 1.00 37.34 | AAAA |
| MOTA | 1900 | | | A 240 | 21.594 | | | 1.00 39.39 | AAAA |
| MOTA | 1901 | CA | | | 20.281 | | | 1.00 41.90 | AAAA |
| MOTA | 1902 | | GLU | A 240 | 20.040 | | | | AAAA |
| MOTA | 1903 | CG | | A 240 | 19.665 | | | | AAAA |
| ATOM | 1904 | | | A 240 | | | | | AAAA |
| ATOM | 1905 | OE: | | A 240 | 18.670 | | | | AAAA |
| ATOM | 1906 | OE: | | A 240 | 20.364 | | | | AAAA |
| ATOM | 1907 | | | A 240 | 21.583 | | | | AAAA |
| MOTA | 1908 | | GLU | A 240 | 22.224 | | | | AAAA |
| | 1909 | | ILE | A 241 | 20.847 | | | | AAAA |
| ATOM | 1910 | | TI.E | A 241 | 20.75 | 21.95 | | | |
| ATCM | | | | A 241 | 19.91 | 21.994 | | | AAAA |
| MOTA | 1911 | | | A 241 | 19.85 | | 71.287 | | AAAA |
| MOTA | | | 1 77 7 | A 241 | 18.50 | | | 1.00 41.45 | AAAA |
| MOTA | / | | 1 115 | . A 444 A 2/11 | 17.64 | | | | AAAA |
| MOTA | 1914 | CD. | שעוו די | A 241 | 1,.04 | | • | | • |
| | • | | • | | | | | | |

| | | | • | | 50 003 | 1.00 41.66 | AAAA |
|-------|----------|------------|----------------|----------------|------------------|------------|------|
| > mov | 1915 C | ILE A 24 | 11 22.1 | 59 21.424 | , | | |
| MOTA | | ILE A 24 | 22.4 | 45 20.229 | | 1.00 42.10 | AAAA |
| MOTA | 1916 0 | 105 2 24 | · - | | 72.432 | 1.00 41.42 | AAAA |
| MOTA | 1917 N | VAL A 24 | - | | | 1.00 41.23 | AAAA |
| ATOM | 1918 CA | | | | 71.351 | 1.00 40.40 | AAAA |
| ATOM | 1919 CE | VAL A 24 | 25.0 | | | | AAAA |
| | 1920 CC | 1 VAL A 24 | 42 26.5 | 56 22.850 | 71.171 | 1.00 39.25 | |
| MOTA | | 2 VAL A 24 | 24.4 | 38 23.384 | 70.004 | 1.00 39.79 | AAAA |
| ATOM | | | | | 73.298 | 1.00 42.67 | AAAA |
| MOTA | 1922 C | VAL A 24 | •• | | 73.316 | 1.00 41.83 | AAAA |
| MOTA | 1923 0 | VAL A 24 | 42 25.8 | | | 1.00 44.41 | AAAA |
| MOTA | 1924 N | LYS A 24 | 43 25.1 | | 74.318 | | AAAA |
| | 1925 C | | 43 25.9 | 72 22.215 | 75.523 | 1.00 46.51 | |
| ATOM | | | | | 76.522 | 1.00 47.29 | AAAA |
| ATOM | 1926 CI | | • • | | 77.564 | 1.00 48.40 | AAAA |
| MOTA | 1927 C | LYS A 2 | - | | 78.823 | 1.00 48.88 | AAAA |
| MOTA | 1928 CI | | | | 78.380 | 1.00 49.62 | AAAA |
| ATOM | 1929 C | E LYS A 2 | 43 26.3 | | | 1.00 50.11 | AAAA |
| | 1930 N | | 43 25.9 | | 79.505 | 1.00 30.11 | AAAA |
| ATOM | | | 43 25.6 | 539 20.891 | 76.209 | 1.00 47.59 | |
| MOTA | | | 43 26.5 | 37 20.216 | 76.711 | 1.00 48.17 | AAAA |
| ATOM | 1932 0 | LIS A 4 | | | 76.237 | 1.00 48.86 | AAAA |
| ATOM | 1933 N | GLU A 2 | | | 76.877 | 1.00 50.82 | AAAA |
| MOTA | 1934 C. | A GLU A 2 | | | 77.103 | 1.00 52.08 | AAAA |
| MOTA | 1935 C | B GLU A 2 | 44 22.4 | | | 1.00 53.82 | AAAA |
| | 1936 C | | | | 77.829 | 1.00 53.02 | AAAA |
| ATOM | | D GLU A 2 | | 359 20.174 | 78.230 | 1.00 54.49 | |
| ATOM | | | · • • | | 78.595 | 1.00 55.15 | AAAA |
| MOTA | | E1 GLU A 2 | | | 78.200 | 1.00 54.98 | AAAA |
| ATOM | | E2 GLU A 2 | | | 76.033 | 1.00 51.06 | AAAA |
| MOTA | 1940 C | GLU A 2 | | | 76.477 | 1.00 51.68 | AAAA |
| ATOM | 1941 0 | GLU A 2 | 24. | | | 1.00 51.12 | AAAA |
| MOTA | 1942 N | VAL A 2 | 245 . 24. | | 74.820 | 1.00 51.12 | AAAA |
| | | A VAL A 2 | 245 25. | | 73.904 | 1.00 50.08 | AAAA |
| MOTA | | B VAL A 2 | 245 24. | 217 17.263 | 72.677 | 1.00 50.22 | |
| MOTA | | G1 VAL A 2 | | | 71.651 | 1.00 51.07 | AAAA |
| ATOM | | GI VAL A 2 | | | 73.118 | 1.00 50.79 | AAAA |
| ATOM | | G2 VAL A 2 | | | 73.397 | 1.00 49.43 | AAAA |
| ATOM | 1947 C | VAL A 2 | | - · · - | 72.917 | 1.00 48.65 | AAAA |
| ATOM | 1948 | VAL A 2 | 245 27. | | 73.522 | 1.00 48.65 | AAAA |
| ATOM | 1949 N | I PHE A 2 | | 220 18.408 | | 1.00 47.97 | AAAA |
| | | A PHE A 2 | 246 28. | 556 18.552 | 72.982 | 1.00 47.37 | AAAA |
| MOTA | | B PHE A | 246 28. | 420 19.212 | 71.607 | 1.00 46.45 | AAAA |
| MOTA | | | | 553 18.932 | 70.671 | 1.00 45.35 | |
| MOTA | | G PHE A | | 841 17.629 | 70.280 | 1.00 44.13 | AAAA |
| ATOM | | D1 PHE A | - | 291 19.972 | | 1:00 44.40 | AAAA |
| MOTA | 1954 | D2 PHE A | | | | 1.00 43.95 | AAAA |
| ATOM | 1955 (| CE1 PHE A | | | | 1.00 43.47 | AAAA |
| ATOM | 1956 | CE2 PHE A | | 292 19.721 | | 1.00 44.05 | AAAA |
| MOTA | | Z PHE A | 246 31. | 566 18.422 | | 1.00 49.60 | AAAA |
| | | PHE A | | 481 19.383 | | 1.00 48.60 | AAAA |
| MOTA | | | 246 29. | 132 20.501 | 74.239 | 1.00 49.59 | |
| MOTA | | | | 647 18.834 | | 1.00 48.69 | AAAA |
| MOTA | 1300 | M GLU A | | 644 19.578 | | 1.00 49.45 | AAAA |
| ATOM. | . 1961 (| CA GLU A | | | | 1.00 51.91 | AAAA |
| MOTA | 1962 | CB GLU A | | | | 1.00 54.39 | AAAA |
| ATOM | 1963 | CG GLU A | | .257 18.659 | | 1.00 57.34 | AAAA |
| - | | CD GLU A | | .986 17.845 | | | AAAA |
| MOTA | | OE1 GLU A | | .100 18.315 | 76.393 | 1.00 58.48 | |
| ATOM | | | | .877 16.725 | 77.702 | 1.00 57.95 | AAAA |
| MOTA | | | | .807 19.903 | | 1.00 47.39 | AAAA |
| MOTA | 1967 | C GLU A | | | | | AAAA |
| MOTA | 1968 | O GLU A | ' | | | | AAAA |
| MOTA | 1969 | n PRO A | 2.0 | • • | _ | | AAAA |
| | | CD PRO A | 248 31 | .651 22.03 | | | AAAA |
| MOTA | | CA PRO A | | .710 21.61 | | | AAAA |
| MOTA | | | | .063 22.94 | 8 72.01 7 | | |
| ATOM | | CB PRO A | • • • | .604 22.66 | 1 72.178 | 1.00 46.28 | AAAA |
| MOTA | | CG PRO A | 2-10 | .155 21.81 | | 1.00 44.29 | AAAA |
| MOTA | 1974 | C PRO A | | | | | AAAA |
| MOTA | | O PRO A | | | | | аааа |
| MOTA | | N GLU A | | .100 21.36 | | | AAAA |
| | | CA GLU A | 249 37 | .522 21.52 | | | AAAA |
| ATOM | | CB GLU A | | .344 20.46 | | | AAAA |
| ATOM | | | | .960 19.03 | | 1.00 41.32 | |
| ATOM | | CG GLU A | | .825 18.00 | | | AAAA |
| ATOM | 1980 | CD GLU A | 449 30 | .525 10.00 | | | • |

| | | | | | 20 071 | 10 017 | 69.996 | 1.00 41.55 | AAAA |
|------|------|-----|----------|--------|-----------------|--------|----------|------------|------|
| ATOM | 1981 | OE1 | GLU A | 249 | 38.871 | 18.017 | | 1.00 42.49 | AAAA |
| ATOM | 1982 | OE2 | GLU A | 249 | 39.462 | 17.187 | 71.926 | | |
| | 1983 | C | GLU A | | 37.840 | 22.873 | 71.718 | 1.00 38.81 | AAAA |
| ATOM | | | | | 38.715 | 23.617 | 72.181 | 1.00 38.27 | AAAA |
| MOTA | 1984 | 0 | GLU A | | | | 70.644 | 1.00 36.60 | AAAA |
| MOTA | 1985 | N | VAL A | | 37.109 | 23.160 | | 1.00 34.20 | AAAA |
| ATOM | 1986 | CA | VAL A | 250 | 37.242 | 24.402 | 69.890 | | |
| | | CB | VAL A | 250 | 38.379 | 24.321 | 68.862 | 1.00 33.73 | AAAA |
| MOTA | 1987 | | | | 38.085 | 23.209 | 67.864 | 1.00 33.26 | AAAA |
| ATOM | 1988 | | VAL A | | | | | 1.00 33.75 | AAAA |
| ATOM | 1989 | CG2 | VAL A | 1, 250 | 38.546 | 25.678 | 68.153 | | AAAA |
| | 1990 | С | VAL A | | 35.945 | 24.617 | 69.130 | 1.00 31.98 | |
| ATOM | | | VAL A | | 35.205 | 23.658 | 68.904 | 1.00 32.36 | AAAA |
| MOTA | 1991 | 0 | | | | 25.863 | 68.760 | 1.00 28.65 | AAAA |
| ATOM | 1992 | N | TYR A | 1 251 | 35.657 | | | 1.00 26.49 | AAAA |
| ATOM | 1993 | CA | TYR A | 251 | 34.449 | 26.150 | 67.991 | | - |
| | 1994 | CB | TYR A | | 33.241 | 26.442 | 68.906 | 1.00 24.32 | AAAA |
| - | | | TYR A | | 33.193 | 27.853 | 69.465 | 1.00 22.96 | AAAA |
| MOTA | 1995 | CG | | | | 28.931 | 68.668 | 1.00 22.21 | AAAA |
| ATOM | 1996 | CD1 | | | 32.771 | | | 1.00 21.29 | AAAA |
| ATOM | 1997 | CE1 | TYR A | A 251 | 32 <i>.</i> 791 | 30.234 | 69.151 | 1.00 21.29 | |
| | | CD2 | TYR A | | 33.628 | 28.124 | 70.771 | 1.00 21.47 | AAAA |
| MOTA | 1998 | | | | 33.651 | 29.425 | 71.265 | 1.00 20.80 | AAAA |
| MOTA | 1999 | CE2 | TYR A | | | | | 1.00 20.77 | AAAA |
| ATOM | 2000 | CZ | | A 251 | 33.237 | 30.475 | 70.449 | | AAAA |
| ATOM | 2001 | OH | TYR | A 251 | 33.309 | 31.768 | 70.913 | 1.00 21.41 | |
| - | | | | A 251 | 34.691 | 27.345 | 67.092 | 1.00 24.59 | AAAA |
| ATOM | 2002 | С | | | 35.504 | 28.216 | 67.410 | 1.00 25.87 | AAAA |
| ATOM | 2003 | 0 | | A 251 | | | | 1.00 22.49 | AAAA |
| MOTA | 2004 | N | LEU A | A 252 | 33.984 | 27.374 | 65.970 | | AAAA |
| | 2005 | CA | LEU | A 252 | 34.082 | 28.482 | 65.045 | 1.00 20.96 | |
| MOTA | | | 7 511 | A 252 | 34.523 | 28.018 | 63.657 | 1.00 21.31 | AAAA |
| MOTA | 2006 | CB | | | 35.940 | 27,472 | 63.556 | 1.00 21.03 | AAAA |
| MOTA | 2007 | CG | | A 252 | | | | 1.00 22.16 | AAAA |
| MOTA | 2008 | CD1 | LEU A | A 252 | 35.947 | 26.028 | 63.977 | | |
| | 2009 | CD3 | LEU A | A 252 | 36.440 | 27.594 | 62.143 | 1.00 22.13 | AAAA |
| ATOM | - | | T ETT | A 252 | 32.731 | 29.159 | 64.959 | 1.00 19.60 | AAAA |
| MOTA | 2010 | С | | | | 28.523 | 65.070 | 1.00 19.95 | AAAA |
| ATOM | 2011 | 0 | LEU . | A 252 | 31.689 | | | | AAAA |
| ATOM | 2012 | N | LEU . | A 253 | 32.748 | 30.461 | 64.756 | 1.00 17.93 | |
| | 2013 | CA | LEII | A 253 | 31.521 | 31.222 | 64.675 | 1.00 17.33 | AAAA |
| MOTA | | | | A 253 | 31.441 | 32.142 | 65.900 | 1.00 16.31 | AAAA |
| ATOM | 2014 | CB | | | | 33.070 | 66.153 | 1.00 15.81 | AAAA |
| MOTA | 2015 | CG | | A 253 | 30.266 | | | 1.00 14.74 | AAAA |
| ATOM | 2016 | CDI | LEU | A 253 | 28.990 | 32.267 | 66.377 | | |
| | 2017 | CD3 | LEU | A 253 | 30.602 | 33.925 | 67.368 | 1.00 15.83 | AAAA |
| ATOM | | | | A 253 | 31.564 | 32.035 | 63.386 | 1.00 16.60 | AAAA |
| MOTA | 2018 | C | | | | 32.722 | 63.132 | 1.00 16.40 | AAAA |
| ATOM | 2019 | 0 | | A 253 | 32.548 | | | 1.00 15.88 | AAAA |
| ATOM | 2020 | N | GLN | A 254 | 30.526 | 31.936 | 62.557 | | |
| | 2021 | CA | | A 254 | 30.507 | 32.716 | 61.328 | 1.00 16.27 | AAAA |
| MOTA | | | | A 254 | 30.045 | 31.881 | 60.121 | 1.00 15.88 | AAAA |
| MOTA | 2022 | CB | | | | 32.048 | 59.734 | 1.00 18.52 | AAAA |
| ATOM | 2023 | ÇG | | A 254 | 28.587 | | | 1.00 17.54 | AAAA |
| ATOM | 2024 | CD | GLN | A 254 | 28.380 | 32.935 | 58.519 | | |
| | 2025 | OFI | CI.N | A 254 | 28.714 | 32.572 | 57.391 | 1.00 15.89 | AAAA |
| ATOM | | | | | 27.828 | 34.103 | 58.750 | 1 00 18.49 | AAAA |
| MOTA | 2026 | NE2 | GLN | A 234 | | | 61.650 | 1 00 16.91 | AAAA |
| MOTA | 2027 | С | GLN | A 254 | 29.527 | 33.825 | 62.000 | 1 00 17.41 | AAAA |
| ATOM | 2028 | 0 | GLN | A 254 | 28.450 | 33.571 | 62.198 | 1 70 17.41 | |
| | | | TETT | A 255 | 29.911 | 35.053 | 61.319 | 1.00 16.68 | AAAA |
| ATOM | 2029 | N | 1,50 | 222 | 29.102 | 36.215 | 61.619 | 1.00 16.42 | AAAA |
| ATOM | 2030 | CA | LEU | A 255 | | | | | AAAA |
| MOTA | 2031 | CB | LEU | A 255 | 29.861 | 37.080 | | | AAAA |
| | 2032 | CG | T.EU | A 255 | 30.269 | 36.301 | 63.860 | 1.00 13.90 | |
| MOTA | | CD1 | 1 211 | A 255 | 31.494 | 36.924 | 64.515 | 1.00 12.24 | AAAA |
| MOTA | 2033 | CDI | LEU | 255 | | 36.202 | 64.774 | 1.00 12.80 | AAAA |
| MOTA | 2034 | CD2 | LEU | A 255 | 29.083 | | | 1.00 18.32 | AAAA |
| MOTA | 2035 | С | LEU | A 255 | 28.699 | 37.048 | | 1.00 10.52 | AAAA |
| | 2036 | ō | | A 255 | 29.170 | 38.177 | | 1.00 17.59 | |
| ATOM | | | CT 17 | A 256 | 27.813 | 36.482 | | 1.00 19.75 | AAAA |
| MOTA | 2037 | N | لابلق | A 230 | | 37.188 | | 1.00 20.77 | AAAA |
| ATOM | 2038 | CA | | A 256 | 27.322 | | | 1.00 21.73 | AAAA |
| ATOM | 2039 | С | GLY | A 256 | 26.422 | 38.302 | | | |
| | | | | A 256 | 25.642 | 3ø.096 | 59.857 | 1.00 21.38 | AAAA |
| MOTA | 2040 | 0 | | . 250 | 26.528 | 39.485 | | | AAAA |
| ATOM | 2041 | N | | A 257 | | | | | AAAA |
| ATOM | 2042 | CA | THR | A 257 | 25.721 | 40.622 | | | AAAA |
| | 2043 | CB | THR | A 257 | 26.460 | 41.968 | | | |
| MOTA | | | ייייין ו | A 257 | 26.729 | 42.169 | | 1.00 25.54 | AAAA |
| MOTA | 2044 | | 7 1111 | A 257 | 27.780 | 41.985 | | | AAAA |
| MOTA | 2045 | CG: | 2 THR | A 257 | | | | | AAAA |
| MOTA | 2046 | С | THR | A 257 | 24.438 | 40.691 | . 3/.340 | 1.00 22.07 | • |
| | | | | | | | | | - |

| | 2017 | _ | THR A | 257 | 23.692 | 41.672 | | 1.00 25.84 | AAAA |
|--------|--------|-----|---|---------|--------|----------|----------|--------------|------|
| MOTA | | 0 | ASP A | 25. | 24.152 | 39.665 | | 1.00 25.18 | AAAA |
| ATOM | | N | ASP A | 250 | 22.935 | 39.753 | 56.379 | 1.00 26.18 | AAAA |
| MOTA | 2049 | CA | ASP A | 258 | | 38.830 | 55.149 | 1.00 25.52 | AAAA |
| ATOM | 2050 | CB | ASP A | 258 | 22.950 | | 55.494 | 1.00 26.33 | AAAA |
| ATOM | 2051 | CG | ASP A | 258 | 23.211 | 37.392 | | 1.00 26.74 | AAAA |
| ATOM | 2052 | C | ASP A | 258 | 21.649 | 39:574 | 57.178 | | AAAA |
| | | o | ASP A | 258 | 20.571 | 39.823 | 56.643 | 1.00 26.57 | |
| ATOM | 2053. | 001 | ASP A | 258 | 23.014 | 37.029 | 56.675 | 1.00 26.85 | AAAA |
| MOTA | | ODI | ASP A | 250 | 23.585 | 36:623 | 54.572 | 1.00 24.06 | AAAA |
| MOTA | _ | | ASP A | 250 | 21.727 | 39.114 | 58.449 | 1.00 26.95 | AAAA |
| MOTA | 2056 | n | PRO A | . 259 | | 38.589 | 59.271 | 1.00 27.34 | AAAA |
| MOTA | 2057 | CD | PRO A | . 259 - | 22.834 | | 59.190 | 1.00 27.05 | AAAA |
| MOTA | 2058 | CA | PRO A | 259 | 20.467 | 38.976 | | 1.00 26.38 | AAAA |
| ATOM | 2059 | CB | PRO A | 259 | 20.886 | 38.186 | 60.425 | | AAAA |
| | 2060 | CG | PRO A | 259 | 22.247 | 38.718 | 60.669 | 1.00 27.84 | |
| MOTA | _ | C | PRO A | 259 | 19.914 | 40.365 | 59.543 | 1.00 27.32 | AAAA |
| MOTA | 2061 | | PRO A | 250 | 18.739 | 40.510 | 59.871- | 1.00 27.29 | AAAA |
| MOTA | 2062 | 0 | | | 20.771 | 41.383 | 59.452 | 1.00 26.97 | AAAA |
| MOTA | 2063 | N | LEU A | 260 | 20.389 | 42.763 | 59.752 | 1.00 26.74 | AAAA |
| MOTA | 2064 | CA | LEU A | 1 260 | | 43.680 | 59.680 | 1.00 27.21 | AAAA |
| MOTA | 2065 | CB | LEU A | A 260 | 21.621 | | 60.709 | 1.00 27.01 | AAAA |
| ATOM | 2066 | CG | LEU A | 3 260 | 22.732 | 43.465 | | 1.00 25.51 | AAAA |
| ATOM | 2067 | CD1 | LEU A | A 260 | 23.889 | 44.380 | 60.408 | 1.00 27.39 | AAAA |
| | 2068 | CD2 | LEU A | A 260 | 22.189 | 43.718 | 62.112 | 1.00 27.39 | AAAA |
| ATOM | | C | TEII : | A 260 | 19.295 | 43.351 | 58.865 | 1.00 26.47 | |
| MOTA | 2069 | | 7 577 | A 260 | 19.278 | 43.137 | 57.649 | 1.00 26.72 | AAAA |
| MOTA | 2070 | 0 | LEU A | 200 | 18.413 | 44.126 | 59.494 | 1.00 26.32 | AAAA |
| MOTA | 2071 | N | LEU | A 261 | 17.283 | 44.808 | 58.846 | 1.00 27.20 | AAAA |
| MOTA | 2072 | CA | | A 261 | _ | 45.885 | 59.780 | 1.00 28.71 | AAAA |
| MOTA | 2073 | CB | | A 261 | 16.732 | | 59.190 | 1.00 29.24 | AAAA |
| ATOM | 2074 | CG | LEU . | A 261 . | 15.644 | 46.789 | 58.883 | 1.00 29.44 | AAAA |
| ATOM | 2075 | CD1 | LEU 2 | A 261 | 14.433 | 45.954 | | 1.00 29.72 | AAAA |
| ATOM - | 2076 | CD2 | LEU . | A 261 | 15.284 | 47.906 | 60.162 | | AAAA |
| | 2077 | C | LEU | A 261 | 17.506 | | 57.473 | 1.00 27.90 | AAAA |
| ATOM | | | T EII | A 261 | 16.675 | 45.294 | | 1.00 28.21 | |
| MOTA | 2078 | 0 | CIII | A 262 | 18.597 | | 57.310 | 1.00 27.61 | AAAA |
| MOTA | 2079 | N | GLU | A 202 | 18.887 | | | 1.00 26.92 | AAAA |
| MOTA | 2080 | CA | GLU | A 262 · | 19.949 | | | 1.00 25.85 | AAAA |
| ATOM | 2081 | CB | GLU | A 262 | | | | 1.00 25.36 | AAAA |
| ATOM | 2082 | CG | GLU | A 262 | 19.549 | 49.119 | | 1.00 25.78 | AAAA |
| ATOM | 2083 | CD | GLU | A 262 | 19.552 | | | 1.00 24.64 | AAAA |
| ATOM | 2084 | OE1 | GLU | A 262 | 19.859 | | | 1.00 25.82 | AAAA |
| | 2085 | OE2 | GLU | A 262 | 19.255 | | | | AAAA |
| MOTA | 2086 | C | GLII | A 262 | 19.346 | 45.995 | | | AAAA |
| MOTA | | | | A 262 | 19.354 | | | 1.00 28.70 | |
| MOTA | 2087 | 0 | | A 263 | 19.743 | | 55.179 | 1.00 29.57 | AAAA |
| MOTA | 2088 | N | ASP | A 263 | 20.23 | | 54.145 | 1.00 28.99 | AAAA |
| ATOM | 2089 | CA | ASP | A 203 | 21.160 | 42.802 | | 1.00 27.89 | AAAA |
| MOTA | 2090 | CB | ASP | A 263 | 21.98 | | | 1.00 29.02 | AAAA |
| MOTA | 2091 | CG | ASP | A 263 | | | | | AAAA |
| MOTA | 2092 | OD1 | LASP | A 263 | 23.19 | | | | AAAA |
| ATOM | 2093 | OD2 | 2 ASP | A 263 | 21.43 | 8 41.663 | | | AAAA |
| MOTA | 2094 | С | ASP | A 263 | 19.06 | 6 43.19 | | | AAAA |
| | 2095 | ō | ASP | A 263 | 18.25 | 8 42.510 | 54.043 | | AAAA |
| MOTA | | | TVD | A 264 | 19.00 | | | | |
| MOTA | 2096 | N | MAD | A 264 | 17.92 | | B 51.306 | 1.00 32.43 | AAAA |
| ATOM | 2097 | CA | TIK | A 204 | 17.91 | | | 1.00 34.53 | AAAA |
| MOTA | 2098 | CB | TYR | A 264 | | · | | | AAAA |
| MOTA | 2099 | CG | TYR | A 264 | 17.62 | | | | AAAA |
| ATOM | 2100 | CD: | 1 TYR | A 264 | 18.66 | | | | AAAA |
| ATOM | 2101 | CE | 1 TYR | A 264 | 18.40 | | | | AAAA |
| MOTA | 2102 | CD | 2 TYR | A 264 | 16.31 | 6 45.51 | | | AAAA |
| | _ | CE | | A 264 | 16.04 | 4 46.87 | 7 50.191 | 1.00 41.50 | AAAA |
| MOTA | | | TVE | A 264 | 17.09 | 5 47.78 | 6 50.170 | 1.00 42.75 | |
| MOTA | | | * 7 17 | A 264 | 16.83 | | 7 50.231 | | AAAA |
| MOTA | | | TYK | 7 204 | 17.89 | | | 1.00 32.50 | AAAA |
| ATOM | | | TYR | A 264 | | | | 3 1.00 32.49 | AAAA |
| ATOM | 2107 | | TYR | A 264 | 16.81 | | | | AAAA |
| ATOM | | 11 | LEU | A 265 | 19.06 | | - | | AAAA |
| ATOM | | | LEU | A 265 | 19.12 | | | | AAAA |
| | | | LEU | A 265 | 20.52 | | | | AAAA |
| ATOM | | | וות.ו | A 265 | 20.80 | | | | AAAA |
| ATOM | | | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | A 265 | 22.21 | | 8 48.77 | 1 1.00 31.59 | AAAA |
| ATOM | 1 2112 | | اعد بدر | 7 200 | 3 | | - | | • |
| • | | | | | | | | | |

| | | | | | | | 20 166 | 48.361 | 1.00 34.62 | AAAA |
|--------|------|-------|---|--------|---|---------|---------|---------------------|------------|--------|
| ATOM | 2113 | CD2 | LEU A | 265 | | 19.803 | 38.166 | | | |
| | | Ç | LEU F | 265 | | 18.693 | 38.540 | 52.296 | 1.00 30.33 | AAAA |
| MOTA | 2114 | • | | | | 19.024 | 37.375 | 52.484 | 1.00 30.30 | AAAA |
| ATOM | 2115 | 0 | LEU A | | | | | | 1.00 29.23 | AAAA |
| | 2116 | N | SER A | 266 | | 17.945 | 39.230 | 53.147 | | |
| MOTA | | - | CER 7 | 266 | | 17.434 | 38.649 | 54.371 | 1.00 29.72 | AAAA , |
| ATOM | 2117 | CA | SER A | 200 | | | 38.894 | 55.519 | 1.00 32.09 | AAAA |
| ATOM - | 2118 | CB | SER A | 266 | | 18.398 | | | | AAAA |
| | | OG | SER A | 266 | | 17.728 | 38.810 | 56.771 | 1.00 33.43 | |
| MOTA | 2119 | | | | | 16.115 | 39.290 | 54.698 | 1.00 28.71 | ÀAAA |
| MOTA | 2120 | С | SER A | 4 266 | | | | | 1.00 29.67 | AAAA |
| | 2121 | 0 | SER A | A 266 | | 15.924 | 40.473 | 54.444 | | |
| MOTA | | | - 110 | A 267 | | 15.209 | 38.517 | 55.276 | 1.00 27.82 | AAAA |
| MOTA | 2122 | N | LID A | 4 207 | | | | 55.654 | 1.00 27.56 | AAAA |
| ATOM | 2123 | CA | LYS A | A 267 | | 13.908 | 39.045 | _ | | AAAA |
| | | | TVC | A .267 | | 12.821 | 38.076 | 55.222 | 1.00 28.75 | |
| MOTA | 2124 | CB | D13 2 | . 267 | - | 12.733 | 37 922 | 53.718 ⁻ | 1.00 29.67 | AAAA |
| ATOM | 2125 | ÇG | LYS | A 267 | | | | | 1.00 30.13 | AAAA |
| | 2126 | CD | LYS A | A 267 | | 12.343 | 39.223 | 53.053 | 1.00 30.13 | |
| MOTA | | | TVC | A 267 | | 12.303 | 39.036 | 51.546 | 1.00 31.86 | AAAA |
| ATOM | 2127 | CE | LID 4 | A 207 | | | 40.252 | 50.843 | 1.00 33.92 | - AAAA |
| ATOM | 2128 | ΝZ | LYS 2 | A 267 | | 11.796 | | | 1.00 27.18 | AAAA |
| | 2129 | С | LVS | A 267 | | 13.800 | 39.327 | 57.152 | 1.00 27.18 | |
| ATOM | | | | 267 | | 12.707 | 39.591 | 57.665 | 1.00 27.18 | AAAA |
| ATOM | 2130 | 0 | LYS . | A 267 | | | | 57.836 | 1.00 26.12 | AAAA |
| | 2131 | N | PHE . | A 268 | | 14.944 | 39.267 | | 1.00 20.12 | AAAA |
| MOTA | | | DUE | A 268 | | 15.048 | 39.532 | 59.271 | 1.00 25.72 | |
| ATOM | 2132 | CA | PRE | - 200 | | 16.272 | 38.830 | 59.856 | 1.00 24.94 | AAAA |
| ATOM | 2133 | CB | PHE | A 268 | | | | | 1.00 25.07 | AAAA |
| | 2134 | CG | PHE | A 268 | | 16.167 | 37.334 | 59.896 | | |
| MOTA | | | | | | 17.271 | 36.565 | 60.267 | 1.00 24.56 | AAAA |
| MOTA | 2135 | CD1 | PHE | A 268 | | | | 59.629 | 1.00 23.76 | AAAA |
| ATOM | 2136 | CD2 | PHE | A 268 | | 14.955 | 36.687 | | 1.00 23 71 | AAAA |
| | | CE1 | DUE | A 268 | | 17.174 | 35.169 | 60.384 | 1.00 23.71 | |
| MOTA | 2137 | CEL | Pnb | 200 | | 14.850 | 35.303 | 59.739 | 1.00 23.86 | AAAA |
| ATOM | 2138 | CE2 | PHE | A 268 | | | | | 1.00 23.68 | AAAA |
| | 2139 | CZ | PHE | A 268 | | 15.966 | 34.542 | 60.121 | 1.00 25.00 | |
| MOTA | | | DITE | A 268 | | 15.190 | 41.030 | 59.513 | 1.00 25.77 | AAAA |
| ATOM | 2140 | С | PRE | A 200 | | | 41.734 | 58.726 | 1.00 25.81 | AAAA |
| MOTA | 2141 | 0 | PHE | A 268 | | 15.811 | | | 1.00 26.02 | AAAA |
| | 2142 | N | ACN | A 269 | | 14.606 | 41.524 | 60.595 | 1.00 20.02 | |
| MOTA | | - | 7011 | 260 | | 14.718 | 42.943 | 60.890 | 1.00 26.58 | AAAA |
| MOTA | 2143 | CA | ASN | A 269 | | | | 61.058 | 1.00 25.47 | AAAA |
| ATOM | 2144 | CB | ASN | A 269 | | 13.330 | 43.584 | | 1.00 25.37 | AAAA |
| | | | 3 CM | A 269 | | 12.379 | 43.252. | 59.906 | 1.00 25.37 | |
| MOTA | 2145 | CG | ASIV | - 200 | | 12.761 | 43.260 | 58.734 | 1.00 23.82 | AAAA |
| ATOM | 2146 | QD1 | ASN | A 269 | | | | | 1.00 24.03 | AAAA |
| | 2147 | 2חוא | ASN | A 269 | | 11.123 | 42.985 | 60.245 | 1.00 24.00 | |
| ATOM | | | 3 CM | A 269 | | 15.540 | 43.112 | 62.169 | 1.00 26.82 | AAAA |
| MOTA | 2148 | С | ADM | A 203 | | | 43.715 | 63.150 | 1.00 27.98 | AAAA ` |
| MOTA | 2149 | 0 | ASN | A 269 | | 15.089 | | | 1.00 26.07 | AAAA |
| | | N | ा.सा | A 270 | | 16.744 | 42.559 | 62.149 | 1.00 20.07 | |
| MOTA | 2150 | | 220 | A 270 | | 17.639 | 42.642 | 63.289 | 1.00 25.97 | AAAA |
| ATOM | 2151 | CA | LEU | A 2/0 | | | | 63.265 | 1.00 23.76 | AAAA |
| ATOM | 2152 | CB | LEU | A 270 | | 18.634 | 41.479 | | 1.00 23.36 | AAAA |
| | _ | CG | 1 511 | A 270 | | 18.048 | 40.070 | 63.225 | 1.00 23.30 | |
| MOTA | 2153 | | | 270 | | 19.115 | 39.090 | 63.710 | 1.00 21.90 | AAAA |
| MOTA | 2154 | CD3 | LEU | A 270 | | | | | 1.00 22.05 | AAAA |
| MOTA | 2155 | · CD2 | LEU | A 270 | | 16.824 | 39.971 | | 1.00 22.00 | AAAA |
| | | | TEII | A 270 | | 18.420 | 43.961 | 63.360 | 1.00 27.13 | |
| MOTA | 2156 | C | 150 | 270 | | | 44.750 | | 1.00 25.99 | AAAA |
| MOTA | 2157 | 0 | | A 270 | | 18.475 | | | | AAAA |
| | 2158 | N | SER | A 271 | | 19.038 | 44.176 | | 1.00 27.57 | AAAA |
| ATOM | | | 222 | A 271 | | 19.832 | 45.370 | 64.767 | 1.00 27.95 | |
| ATOM | 2159 | CA | SEK | 2 2/1 | | | 46.137 | | | AAAA |
| ATOM | 2160 | CB | SER | A 271 | | 19.235 | | | | AAAA |
| | | OG | SER | A 271 | | 19.184 | 45.297 | 67.089 | 1.00 27.50 | |
| ATOM | 2161 | | ~==, | A 271 | | 21.276 | 44.987 | | 1.00 28.15 | AAAA |
| ATOM | 2162 | C | SER | A 271 | | | | | | AAAA |
| ATOM | 2163 | 0 | SER | A 271 | | 21.574 | 43.832 | | | AAAA |
| | | | 3 CM | A 272 | | 22.156 | 45.980 | 64.979 | 1.00 28.96 | |
| MOTA | 2164 | N | ASIN | 7 272 | | | 45.861 | | 1.00 29.54 | AAAA |
| MOTA | 2165 | CA | ASN | A 272 | | 23.590 | | | | AAAA |
| | 2166 | | ASN | A 272 | | 24.247 | 47.243 | | | |
| ATOM | | | | 277 | | 24.647 | 47.640 | 63.850 | 1.00 31.20 | AAAA |
| MOTA | 2167 | | | A 272 | | | | | | AAAA |
| ATOM | 2168 | OD | 1 ASN | A 272 | | 24.960 | 48.794 | | | AAAA |
| | | _ | | A 272 | | 24.670 | 46.674 | 62.948 | | |
| ATOM | 2169 | | ~ Y2W | 7 2/2 | | | 45.309 | | 1.00 29.63 | AAAA |
| MOTA | 2170 | С | ASN | A 272 | | 23.821 | | | | AAAA |
| | 2171 | | ASN | A 272 | | .24.574 | 44.361 | | | |
| MOTA | | | | | | 23.180 | 45.959 | 67.600 | 1.00 29.77 | AAAA |
| MOTA | 2172 | | VAL | A 273 | | 23.100 | | | | AAAA |
| ATOM | 2173 | CA | VAL | A 273 | | 23.290 | 45.602 | | | AAAA |
| | | | 1727 | A 273 | | 22.436 | 46.576 | | | |
| atom | 2174 | | VAL | 2 272 | | 22.716 | _ | | 1.00 33.17 | AAAA |
| MOTA | 2175 | CG | 1 VAL | A 273 | - | | | | | AAAA |
| | | | 2 VAT | A 273 | | 22.740 | | | | AAAA |
| ATOM | | | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | A 272 | | 22.883 | | 4 69.266 | 1.00 30.74 | |
| MOTA | 2177 | | VAL | A 273 | | | | . | | AAAA |
| MOTA | | 3 0 | VAL | A 273 | | 23.550 | 43.43 | , 0.024 | | • |

| | | | | | _ | | | | | | | | | | | |
|--------------|--------------|----------|----------------|----------------|---|----------------|-----|------|----------------|-----|----------------|-----|-------|-----------|--------------|--------------|
| | | | | 271 | 2 | 1.789 | 5 4 | 13.1 | 706 | 68. | 659 | 1.0 | 0 3 | 30. | 25 | AAAA |
| MOTA | 2179 | N | ALA A ALA A | 274 | | 1.32 | | 12. | | 68. | | 1.0 | 0 2 | 29. | 87 | AAAA |
| MOTA | 2180 | CA CB | ALA A | 274 | | 0.00 | | 12. | | 68. | 112 | 1.0 | 0 2 | 29. | 64 | AAAA |
| MOTA | 2181 | CB | ALA A | 274 | 2 | 2.39 | 5 4 | 41.4 | 438 | 68. | 247 | 1.0 | 0 2 | 29. | 35 | AAAA |
| MOTA | 2182 | С 0 | ALA A | 274 | | 2.70 | | 40.3 | 373 | 68. | 778 | 1.0 | 0 2 | 29. | 18 | AAAA |
| ATOM | 2183 2184 | N | PHE A | 275 | 2 | 2.94 | 6 4 | 41. | 893 | 67. | | 1.0 | 0 2 | 29. | 30 | AAAA |
| ATOM | 2185 | CA | PHE A | 275 | | 3.99 | | 41. | 170 | 66. | | 1.0 | 0 3 | 28. | 91 | AAAA |
| MOTA | 2186 | CB | PHE A | 275 | 2 | 4.37 | 5 4 | 41. | 909 | 65. | | 1.0 | 0 2 | 28. | .77 | AAAA |
| ATOM | 2187 | CG | PHE A | 275 | 2 | 5.35 | | 41. | | 64. | | 1.0 | 0 | 28. | 80. | AAAA AAAA |
| MOTA MOTA | 2188 | CD1 | PHE A | 275 | | 5.01 | - | 39. | | 63. | | 1.0 | 0 . | 28. 20 | .92 | AAAA |
| ATOM | 2189 | CD2 | PHE A | 275 | _ | 6.62 | | 41. | | 64. | | 1.0 | 0 | 23. 20 | .40 20 | AAAA |
| MOTA | 2190 | CE1 | PHE A | 275 | | 5.92 | | | 259 | 62. | | 1.0 | 0 | 23. 20 | 24 | AAAA |
| ATOM | 2191 | CE2 | PHE A | 275 | | 7.54 | | | 988 | | 279 716 | 1.0 | 10 | 23. 28 | .30 | AAAA |
| ATOM | 2192 | CZ | PHE A | 275 | | 7.19 | - | | 779 058 | | 351 | 1.0 | 0 | 27 | . 64 | AAAA |
| ATOM | 2193 | С | PHE A | 275 | | 5.19 | - | | 975 | | 558 | 1.0 | 0 | 28 | .65 | AAAA |
| MOTA | 2194 | 0 | PHE A | 275 | | 5.72 5.60 | | | 189 | | 902 | 1.0 | 00 | 26 | .81 | AAAA |
| MOTA | 2195 | N | LEU A | 276 | | 26.73 | - | | 260 | | 831 | 1.0 | 00 | 27 | .38 | AAAA |
| MOTA | 2196 | CA | LEU A | 276 | | 26.87 | | | 700 | | 353 | | | | .53 | AAAA |
| MOTA | 2197 | CB | LEU A | 276 | | 28.20 | | | 213 | | 928 | 1.0 | 00 | 26 | .37 | AAAA |
| MOTA | 2198 | CG | LEU A | 276 | | 7.92 | | | 488 | 70. | 721 | 1.0 | 00 | 25 | .71 | AAAA |
| MOTA | 2199 | CDI | LEU A | 276 | | 28.84 | | | 189 | 70. | 827 | 1.0 | 00 | 27 | .06 | AAAA |
| ATOM | 2200 | CDZ | LEU A | 276 | | 26.48 | | | 317 | | .021 | 1. | 00 | 26 | .49 | AAAA |
| ATOM | 2201 2202 | 0 | LEU A | 276 | | 27.38 | 7 | | 603 | | 471 | 1. | 00 | 25 | .26 | AAAA |
| MOTA MOTA | 2202 | N | LYS A | | : | 25.25 | 7 | | 322 | | .524 | 1. | 00 | 27 | .46 | AAAA AAAA |
| ATOM | 2204 | CA | LYS A | A 277 | | 24.89 | | | 468 | | . 642 | | | | . 63 | AAAA |
| ATOM | 2205 | СВ | LYS A | a 277 | | 23.54 | | | . 862 | | . 223 | 1. | 00 | 20 | .63 .14 | AAAA |
| ATOM | 2206 | CG | | A 277 | | 23.59 | | | . 029 | | .153 .268 | 1 | 00 | 34 | .94 | AAAA |
| ATOM | 2207 | CD | | A 277 | | 22.59 | | | .791 | | .029 | 1 | 00 | 36 | .17 | AAAA |
| ATOM | 2208 | CE | LYS | A 277 | | 22.96 | | | .519 .194 | | .104 | | | | .64 | AAAA |
| MOTA | 2209 | NZ | LYS | A 277 | | 21.97 24.84 | | | .997 | | .297 | ī. | 00 | 28 | .53 | AAAA |
| ATOM | 2210 | С | LYS | A 277 | | 24.0. 25.1 | | | .152 | | .146 | | | | .45 | AAAA |
| MOTA | 2211 | 0 | LYS | A 277 A 278 | | 24.40 | | | .681 | | .064 | 1. | 00 | 28 | 3.47 | AAAA |
| MOTA | 2212 | N | ALA . | A 278 | | 24.4 | | | .280 | 69 | .656 | 1. | 00 | 27 | .66 | AAAA |
| MOTA | 2213 | CA CB | ALA | A 278 | | 23.9 | | | .181 | | .201 | 1. | 00 | 26 | .40 | AAAA |
| MOTA | 2214 2215 | C | ΔΙ.Δ | A 278 | | 25.8 | | 36 | .754 | 69 | .820 | 1. | 00 | 26 | .63 | AAAA |
| MOTA | 2215 | ō | ALA | A 278 | | 26.0 | 81 | | .644 | | .317 | 1. | 00 | 25 | 5.19 | AAAA AAAA |
| ATOM ATOM | 2217 | N | PHE | A 279 | | 26.7 | | | .616 | | .427 | 1. | 00 | 20 | 5.50 5.83 | AAAA |
| ATOM | 2218 | CA | PHE | A 279 | | 28.1 | | | .345 | | .481 | 1. | 00 | 2.5 | 5.35 | AAAA |
| ATOM | 2219 | CB | PHE | A 279 | | 28.9 | | | .521 | | .869 .796 | 1 | 00 | 2 | 7.92 | AAAA |
| ATOM | 2220 | CG | | A 279 | | 30.4 | | | .319 | | .072 | 1 | 00 | 28 | 3.58 | AAAA |
| MOTA | 2221 | CDI | PHE | A 279 | | 30.9 | | | .201 | | .434 | 1. | 00 | - 21 | B.33 | AAAA |
| MOTA | 2222 | CD2 | PHE | A 279 | | 32.3 | | | .078 | | .983 | 1. | 00 | 21 | 8.22 | AAAA |
| MOTA | 2223 | CE | PHE | A 2/9 | | 32.6 | | | .030 | | .349 | 1. | .00 | 21 | 8.11 | AAAA |
| MOTA | 2224 | | PHE | A 279 | | 33.1 | | | .968 | | .622 | 1. | .00 | 2 | 8.21 | AAAA |
| MOTA | 2225 | CZ | PNE | A 279 | | 28.6 | 65 | | .118 | 70 | .901 | 1 | . 00 | 2. | 5.47 | AAAA |
| MOTA | 2226 | С 0 | DHE | A 279 | | 29.2 | | 36 | .091 | 71 | 202 | 1 | .00 | 2 | 4.32 | AAAA |
| MOTA | 2227 2228 | | ASN | A 280 | | 28.3 | | 38 | .075 | | 778 | 1 | .00 | 2 | 5.12 | AAAA |
| ATOM | 2229 | | | A 280 | | 28.8 | 41 | 37 | .944 | | 1.147 | 1 | .00 | 2 | 5.05 | AAAA AAAA |
| MOTA MOTA | 2230 | | ASN | A 280 | | 28.7 | 80 | | .269 | | 3.887 | 1 | .00 | 2 | 4.42 | AAAA |
| MOTA | 2231 | | ASN | A 280 | | 29.6 | 83 | | .300 | | 3.364 | | . 00 | . 2 | 4.56 3.24 | AAAA |
| ATOM | 2232 | | 1 ASN | A 280 | | 30.8 | 41 | | .980 | | 3.080 | | . oc | 1 2 | 4.59 | AAAA |
| ATOM | 2233 | | 2 ASN | A 280 | | 29.2 | | | .543 | | 3.249 | | . ინ | 2 | 4.79 | AAAA |
| ATCM | 2234 | | ASN | A 280 | | 28.2 | | | 814 | _ | 3.925 | | . o c |) 2 | 4.96 | AAAA |
| ATOM | 2235 | | ASN | A 280 | | 28.8 | | | 5.272 | | 1.825 3.565 | | .00 | 2 | 4.87 | AAAA |
| MOTA | 2236 | | ILE | A 281 | | 26.9 | | | 5.444 5.337 | | 4.220 | | .00 | 2 | 4.80 | AAAA |
| ATOM | 2237 | | | A 281 | | 26.3 | | 25 | 5.252 | | 3.780 | | | | 4.40 | AAAA |
| ATOM | 2238 | CB | | A 281 | | 24.8 | | | 3.232 3.907 | | 4.124 | | .00 | 2 | 5.03 | AAAA |
| MOTA | 2239 | | 2 ILE | A 281 | | 24.2 | | | 6.386 | _ | 4.424 | . 1 | .00 |) 2 | 4.70 | AAAA |
| MOTA | 2240 | | 1 ILE | A 281 | | 24.6 | | | 6.379 | | 4.069 | 1 | .00 | 0 2 | 6.49 | AAAA |
| ATOM | 2241 | | 1 ILE | A 281 | | 27.0 |)44 | | 4.027 | | 3.884 | 1 | .00 | 0 2 | 5.21 | AAAA |
| ATOM | | | | A 281 | | 27. | 220 | | 3.170 | | 4.750 |) 1 | .00 | 0 2 | 4.97 | AAAA |
| ATOM | | | | A 281 A 282 | | 27. | | | 3.866 | _ | 2.620 | | .0 | 0 2 | 25.98 | AAAA |
| A TOM | 2244 | N I | سلج | A 404 | | | | ~ . | | - | | | | | | • |

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| | | | | | • | | 100 | 1 00 05 15 | 3335 |
|------|------|-------|-------|-------|--------|----------|--------|------------|--------|
| ATOM | 2245 | CA | VAL A | 282 | 28.150 | 32.656 | 72.193 | 1.00 25.15 | AAAA |
| | 2246 | CB | VAL A | 282 | 28.451 | 32.666 | 70.677 | 1.00 23.83 | AAAA |
| MOTA | | | VAL A | | 29.315 | 31.470 | 70.311 | 1.00 23.58 | AAAA |
| MOTA | 2247 | CGI | VAL | 202 | 27.173 | 32.633 | 69.899 | 1.00 22.73 | AAAA |
| MOTA | 2248 | CG2 | VAL A | 282 | | | 72.936 | 1.00 25.73 | AAAA |
| ATOM | 2249 | | VAL A | | 29.478 | | | 1.00 25.31 | AAAA |
| ATOM | 2250 | 0 . | VAL A | 282 | 29.928 | | 73.275 | | AAAA |
| ATOM | 2251 | | ARG A | 283 | 30.100 | | 73.176 | 1.00 26.90 | |
| | 2252 | | ARG A | | 31.372 | 33.760 | 73.885 | 1.00 28.87 | AAAA |
| ATOM | _ | | ARG A | | 32.027 | | 73.684 | 1.00 28.16 | AAAA |
| MOTA | 2253 | | | | 32.364 | | 72.240 | 1.00 27.22 | AAAA |
| ATOM | 2254 | | ARG A | | | | 72.098 | 1.00 27.08 | AAAA |
| ATOM | 2255 | | ARG A | | 32.821 | | | 1.00 26.73 | AAAA |
| ATOM | 2256 | NE | ARG A | 4 283 | 34.035 | | 72.854 | | AAAA |
| ATOM | 2257 | CZ | ARG A | 283 | 34.514 | 38.327 | 73.091 | 1.00 26.82 | |
| | 2258 | | ARG A | | 33.873 | 39.384 | 72.626 | 1.00 27.36 | AAAA |
| MOTA | | MELO. | ARG A | 283 | 35.622 | 38.484 | 73.798 | 1.00 26.95 | AAAA |
| ATOM | 2259 | | ARG A | . 203 | 31.183 | | 75.376 | 1.00 30.71 | AAAA |
| MOTA | 2260 | С | ARG A | 1 203 | 32.086 | | 76.027 | 1.00 30.68 | AAAA |
| MOTA | 2261 | 0 | ARG A | A 283 | | | 75.911 | 1.00 32.71 | AAAA |
| MOTA | 2262 | N | GLU A | A 284 | 30.014 | | | 1.00 35.53 | AAAA |
| ATOM | 2263 | CA | GLU A | A 284 | 29.735 | | 77.323 | | AAAA |
| ATOM | 2264 | CB | GLU A | A 284 | 28.482 | | 77.751 | 1.00 37.39 | |
| | 2265 | CG | | A 284 | 28.538 | 35.854 | 77.392 | 1.00 41.73 | AAAA |
| MOTA | | | | A 284 | 27.272 | 36.631 | 77.754 | 1.00 45.27 | AAAA |
| MOTA | 2266 | CD | | | 26.151 | | 77.610 | 1.00 46.66 | AAAA |
| MOTA | 2267 | | | A 284 | 27.405 | | 78.148 | 1.00 46.94 | AAAA |
| ATOM | 2268 | OE2 | | A 284 | _ | | 77.564 | 1.00 36.25 | - AAAA |
| MOTA | 2269 | С | GLU A | A 284 | 29.524 | | | 1.00 37.85 | AAAA |
| ATOM | 2270 | 0 | GLU A | A 284 | 29.920 | | 78.601 | | AAAA |
| ATOM | 2271 | N | VAL . | A 285 | 28.916 | 31.464 | 76.591 | 1.00 35.24 | |
| | 2272 | CA | | A 285 | 28.63 | 7 30.041 | 76.708 | 1.00 33.88 | AAAA |
| ATOM | | CB | | A 285 | 27.509 | 29.619 | 75.737 | 1.00 33.71 | AAAA |
| MOTA | 2273 | | | | 27.20 | | 75.888 | 1.00 32.59 | AAAA |
| ATOM | 2274 | CGT | VAL | A 285 | 26.25 | | 76.001 | 1.00 32.77 | AAAA |
| ATOM | 2275 | CG2 | | A 285 | | | 76.456 | 1.00 33.47 | AAAA |
| MOTA | 2276 | С | | A 285 | 29.84 | | | 1.00 34.23 | AAAA |
| MOTA | 2277 | 0 | VAL | A 285 | 30.14 | | 77.257 | | AAAA |
| ATOM | 2278 | N | | A 286 | 30.56 | | 75.364 | 1.00 32.34 | |
| | 2279 | CA | | A 286 | 31.70 | 5 28.535 | 75.036 | 1.00 29.92 | AAAA |
| MOTA | | | | A 286 | 31.53 | 3 27.960 | 73.635 | 1.00 29.77 | AAAA |
| ATOM | 2280 | CB | | | 30.26 | | 73.444 | 1.00 28.64 | AAAA |
| ATOM | 2281 | CG | | A 286 | 29.15 | | 72.863 | 1.00 28.75 | AAAA |
| MOTA | 2282 | CD1 | PHE | A 286 | | | 73.827 | 1.00 28.55 | AAAA |
| MOTA | 2283 | CD2 | PHE | A 286 | 30.19 | | | 1.00 29.04 | AAAA |
| MOTA | 2284 | CE1 | PHE | A 286 | 27.98 | | 72.660 | 1.00 28.19 | AAAA |
| ATOM | 2285 | CE2 | PHE | A 286 | 29.03 | | 73.629 | 1.00 20.19 | AAAA |
| | 2286 | CZ | PHE | A 286 | 27.92 | | | 1.00 28.73 | |
| ATOM | 2287 | C | | A 286 | 33.10 | 6 29.113 | 75.132 | 1.00 29.13 | AAAA |
| ATOM | | | DAE | A 286 | 34.07 | | 74.760 | 1.00 28.54 | AAAA |
| MOTA | 2288 | 0 | PAL | A 200 | 33.22 | | | 1.00 28.42 | AAAA |
| ATOM | 2289 | N | GLX | A 287 | 34.52 | | | 1.00 27.07 | AAAA |
| MOTA | 2290 | CA | GLY | A 287 | | | | 1.00 26.64 | AAAA |
| ATOM | 2291 | С | GLY | A 287 | 34.93 | | | 1.00 27.13 | AAAA |
| MOTA | 2292 | 0 | GLY | A 287 | 34.08 | | | 1.00 27.13 | AAAA |
| MOTA | 2293 | N | GLU | A 288 | 36.22 | | | 1.00 27.20 | AAAA |
| | 2294 | CA | GLU | A 288 | 36.71 | 9 32.238 | 72.900 | 1.00 27.52 | |
| MOTA | | | CTI | A 288 | 38.07 | | 73.108 | 1.00 28.18 | AAAA |
| MOTA | 2295 | CB | GLU | A 200 | 38.03 | | | 1.00 28.88 | AAAA |
| ATOM | 2296 | CG | | A 288 | 37.32 | 9 35.330 | | 1.00 29.58 | AAAA |
| ATOM | 2297 | CD | | A 288 | | | | 1.00 29.94 | AAAA |
| MOTA | 2298 | OE1 | GLU | A 288 | 37.80 | | | | AAAA |
| ATOM | 2299 | OE2 | GLU | A 288 | 36.28 | 1 35.761 | | | |
| | 2300 | C | GLU | A 288 | 36.87 | 7 31.158 | | | AAAA |
| MOTA | | | | A 288 | 37.16 | 9 30.007 | 72.162 | 1.00 27.87 | AAAA |
| ATOM | 2301 | 0 | | | 36.66 | | | 1.00 26.55 | AAAA |
| MOTA | 2302 | N | | A 289 | | | | | AAAA |
| ATOM | 2303 | CA | GLY | A 289 | 36.79 | | | | AAAA |
| ATOM | 2304 | С | GLY | A 289 | 37.28 | | | | AAAA |
| ATOM | 2305 | Ō | GLY | A 289 | 37.63 | | | | AAAA |
| | 2306 | | | A 290 | 37.32 | 0 30.765 | | | |
| MOTA | | | 177.7 | A 290 | 37.75 | | | 1.00 23.76 | AAAA |
| MOTA | 2307 | | ميم. | 3 200 | 38.28 | | | 1.00 24.94 | AAAA |
| ATOM | 2308 | | | A 290 | - | | | | AAAA |
| MOTA | 2309 | CG | L VAL | A 290 | 38.83 | | | | AAAA |
| MOTA | 2310 | CG | VAL | A 290 | 39.37 | 75 29.50 | 00.00 | 1.00 24.73 | • |
| | | | | | | | | | |

| | | | | ` | | | | | • |
|--------------|--------------|---------|---------|------------|--------|------------------|------------------|--------------------------|--------------|
| | | _ | VAL A 2 | 000 | 36.536 | 32.122 | 65.277 | 1.00 23.90 | AAAA |
| ATOM | 2311 | C | VAL A 2 | 200 | 35.497 | 31.502 | 65.100 | 1.00 25.15 | AAAA |
| ATOM | 2312 | • | TÝR A 2 | | 36.662 | 33.415 | 64.976 | 1.00 23.09 | AAAA |
| ATOM | 2313 | | TYR A 2 | | 35.544 | 34.211 | 64.446 | 1.00 21.41 | AAAA |
| MOTA | 2314 | CA | TYR A 2 | 001 | 35.472 | 35.540 | 65.193 | 1.00 20.57 | AAAA |
| ATOM | 2315 | | | | 35.511 | 35:346 | 66.677 | 1.00 19.87 | AAAA |
| MOTA | 2316 | CG | TYR A 2 | 291 | 36.596 | 35.782 | 67.432 | 1.00 20.86 | AAAA |
| ATOM | 2317. | CD1 | TYR A 2 | 291 | 36.677 | 35.513 | 68.793 | 1.00 21.47 | AAAA |
| MOTA | 2318 | | TYR A 2 | | 34.509 | 34:647 | 67.318 | 1.00 20.90 | AAAA |
| MOTA | 2319 | | TYR A 2 | | 34.579 | 34.372 | 68.675 | 1.00 21.90 | AAAA |
| MOTA | 2320 | | TYR A 2 | | 35.661 | 34.800 | 69.403 | 1.00 21.25 | AAAA |
| MOTA | 2321 | CZ | TYR A | | 35.737 | 34.469 | 70.730 | 1.00 23.75 | AAAA |
| MOTA | 2322 | OH | TYR A | | 35.607 | 34.483 | 62.946 | 1.00 21.25 | AAAA |
| MOTA | 2323 | C | TYR A | | 36.573 | 35.077 | 62.451 | 1.00 21.10 | AAAA |
| MOTA | 2324 | 0 | TYR A 2 | | 34.557 | 34.084 | 62.231 | 1.00 20.92 | AAAA |
| MOTA | 2325 | N | LEU A | | 34.518 | 34.260 | 60.779- | 1.00 20.92 | AAAA |
| ATOM | 2326 | CA | LEU A | | 34.235 | 32.916 | 60.080 | 1.00 19.93 | AAAA |
| MOTA | 2327 | CB | LEU A | | 35.104 | 31.688 | 60.399 | 1.00 17.31 | AAAA |
| MOTA | 2328 | CG | LEU A | | 34.685 | 30.515 | 59.528 | 1.00 16.05 | AAAA |
| ATOM | 2329 | | LEU A | | 36.552 | 32.000 | 60.163 | 1.00 18.07 | AAAA |
| MOTA | 2330 | | LEU A | 292 | 33.515 | 35.288 | 60.283 | 1.00 21.12 | AAAA |
| ATOM | 2331 | C | LEU A | | 32.652 | 35.741 | 61.020 | 1.00 20.70 | AAAA |
| MOTA | 2332 | 0 | GLY A | 222 | 33.660 | 35.660 | 59.017 | 1.00 21.74 | AAAA |
| ATOM | 2333 | N | GLY A | | 32.752 | 36.612 | 58.410 | 1.00 21.48 | AAAA |
| ATOM | 2334 | CA | GLY A | | 31.612 | 35.856 | 57.770 | 1.00 21.65 | AAAA |
| MOTA | 2335 | C | GLY A | | 31.237 | 34.790 | 58.235 | 1.00 22.25 | AAAA |
| MOTA | 2336 | 0 | GLY A | | 31.060 | 36.392 | 56.691 | 1.00 22.66 | AAAA |
| MOTA | 2337 | N CA | GLY A | 294 | 29.957 | 35.714 | 56.034 | 1.00 23.61 | AAAA |
| MOTA | 2338 2339 | CA | GLY A | 294 | 29.180 | 36.653 | 55.146 | 1.00 24.56 | AAAA |
| ATOM | | 0 | GLY A | | 29.679 | 37.727 | 54.790 | 1.00 25.54 | AAAA |
| ATOM - | 2340 2341 | N | GLY A | | 27.956 | 36.265 | 54.794 | 1.00 24.06 | AAAA |
| ATOM | 2341 | CA | GLY A | | 27.139 | 37.093 | 53.927 | 1.00 22.78 | AAAA |
| MOTA | 2342 | C | GLY A | 295 | 26.902 | 38.479 | 54.483 | 1.00 23.11 | AAAA |
| MOTA | 2344 | 0. | GLY A | 295 | 26.870 | 38.676 | 55.696 | 1.00 22.87 | AAAA |
| MOTA | 2345 | N. | GLY A | 296 | 26.733 | 39.442 | 53.584 | 1.00 22.78 | AAAA |
| MOTA MOTA | 2346 | CA | GLY A | | 26.497 | 40.813 | 53.993 | 1.00 23.44 | AAAA AAAA |
| ATOM | 2347 | C | GLY A | | 26.471 | 41.618 | 52.718 | 1.00 23.72 | AAAA |
| MOTA | 2348 | ŏ | GLY A | 296 | 27.474 | 41.661 | 52.004 | 1.00 23.73 | AAAA |
| ATOM | 2349 | N | TYR A | 297 | 25.356 | 42.280 | 52.425 | 1.00 23.41 | AAAA |
| ATOM | 2350 | CA | TYR A | 297 | 25.282 | 42.991 | 51.163 | 1.00 22.71 1.00 21.55 | AAAA |
| MOTA | 2351 | CB | TYR A | 297 | 24.252 | 42.294 | 50.296 | 1.00 21.33 | AAAA |
| MOTA | 2352 | CG | TYR A | 297 | 24.496 | 40.809 | 50.317 | 1.00 20.95 | AAAA |
| ATOM | 2353 | CD1 | TYR A | 297 | 24.036 | 40.016 | 51.375 | 1.00 20.55 | AAAA |
| MOTA | 2354 | CE1 | TYR A | 297 | 24.400 | 38.678 | 51.481 49.358 | 1.00 21.71 | AAAA |
| MOTA | 2355 | CD2 | TYR A | 297 | 25.320 | 40.217 | 49.358 | 1.00 21.71 | AAAA |
| MOTA | 2356 | CE2 | TYR A | 297 | 25.688 | 38.900 | 50.511 | 1.00 22.18 | AAAA |
| MOTA | 2357 | CZ | TYR A | 297 | 25.242 | 38.127 36.841 | 50.615 | 1.00 21.35 | AAAA |
| MOTA | 2358 | OH | TYR A | 297 | 25.721 | | 51.225 | 1.00 22.90 | AAAA |
| MOTA | 2359 | С | TYR A | 297 | 25.042 | 44.485 | 50.203 | 1.00 23.17 | AAAA |
| ATOM | 2360 | 0 | TYR A | 297 | 25.106 | 45.172 | 52.417 | | AAAA |
| MOTA | 2361 | N | HIS A | | 24.772 | 44.989 | 52.566 | 1.00 24.27 | AAAA |
| ATOM | 2362 | CA | HIS A | 298 | 24.572 | 46.415 46.726 | 53.556 | | AAAA |
| ATOM | 2363 | CB | HIS A | 298 | 23.468 | | 53.572 | | AAAA |
| MOTA | 2364 | CG | HIS A | 298 | 23.097 | 49.201 | 54.287 | | AAAA |
| MOTA | 2365 | CD2 | HIS A | 298 | 23.588 | 48.708 | | | AAAA |
| ATOM | 2366 | ND: | L HIS A | 298 | 22.199 | | | | AAAA |
| ATOM | 2367 | | L HIS A | | 22.151 | 50.017 50.342 | | | AAAA |
| ATOM | 2368 | | HIS A | 298 | 22.986 | | | | AAAA |
| MOTA | 2369 | С | HIS A | 298 | 25.886 | | | | AAAA |
| ATOM | 2370 | 0 | HIS A | 298 | 26.282 | | | | AAAA |
| ATOM | 2371 | N | PRO A | | 26.563 | | | | AAAA |
| ATOM | 2372 | | PRO A | | 26.178 | | | | AAAA |
| MOTA | 2373 | CA | PRO A | 299 | 27.840 | | | | AAAA |
| ATOM | 2374 | | PRO A | 299 | 28.156 | 49.383 | | | AAAA |
| ATOM | 2375 | CG | PRO A | 299 | 26.743 | 49.764 | | | AAAA |
| ATCM | 2376 | C | PRO A | 299 | 27.824 | 49.037 | . 24.142 | , 1.00 0, | • |
| | | | | | | | | | |

| | | | | | _ | - | | | | |
|--------|--------|-----|--------|-------|---|--------|------------------|------------------|------------|-------|
| | | | | 200 | | 28.755 | 48.826 | 54.939 | 1.00 28.04 | AAAA |
| MOTA | 2377 | | PRO P | 299 | | 26.769 | 49.794 | 54.452 | 1.00 27.04 | AAAA |
| MOTA | 2378 | N | TYR A | 300 | | | 50.477 | 55.740 | 1.00 27.59 | AAAA |
| MOTA | 2379 | CA | TYR A | 300 | | 26.629 | 51.437 | 55.700 | 1.00 30.57 | AAAA |
| ATOM | 2380 | CB | TYR A | | | 25.425 | | 54.718 | 1.00 32.91 | AAAA |
| MOTA | 2381 | CG | | A 300 | | 25.516 | 52.599 | | 1.00 33.45 | AAAA |
| ATOM - | 2382 | CD1 | TYR A | A 300 | | 26.181 | 52.464 | 53.491 | 1.00 33.43 | AAAA |
| ATOM | 2383 | CE1 | TYR A | A 300 | | 26.160 | 53.487 | 52.538 | | AAAA |
| MOTA | 2384 | CD2 | | A 300 | | 24.837 | 53.801 | 54.969 | 1.00 34.19 | AAAA |
| | 2385 | CE2 | | A 300 | | 24.809 | 54.830 | 54.018 | 1.00 34.64 | |
| MOŢA | 2386 | CZ | | A 300 | | 25.468 | 54.657 | 52.807 | 1.00 34.56 | AAAA |
| MOTA | | OH | TVR | A 300 | | 25.389 | 55.630 | 51.844 | 1.00 36.05 | AAAA |
| ATOM | 2387 | | TIN I | A 300 | | 26.454 | 49.538 | 56.936 | 1.00 26.48 | AAAA |
| ATOM | 2388 | C | myp : | A 300 | - | 27.073 | 49.726 | 57.979 - | 1.00 25.81 | AAAA |
| MOTA | 2389 | 0 | TIK | A 301 | | 25.581 | 48.547 | 56.791 | 1.00 25.41 | AAAA |
| MOTA | 2390 | N | ALA A | N 301 | | 25.328 | 47.606 | 57.865 | 1.00 24.64 | AAAA |
| MOTA | 2391 | CA | ALA | A 301 | | 24.164 | 46.731 | 57.511 | 1.00 25.32 | -AAAA |
| ATOM | 2392 | CB | ALA | A 301 | | 26.568 | 46.775 | 58.067 | 1.00 25.53 | AAAA |
| MOTA | 2393 | С | ALA . | A 301 | | | 46.567 | 59.194 | 1.00 26.39 | AAAA |
| ATOM | 2394 | 0 | ALA . | A 301 | | 27.030 | 46.304 | 56.950 | 1.00 25.83 | AAAA |
| MOTA | 2395 | N | LEU . | A 302 | | 27.108 | | 56.926 | 1.00 26.32 | AAAA |
| ATOM | 2396 | CA | | A 302 | | 28.323 | 45.500 | 55.479 | 1.00 27.38 | AAAA |
| ATOM | 2397 | CB | | A 302 | | 28.782 | 45.378 | | 1.00 28.18 | AAAA |
| MOTA | 2398 | CG | | A 302 | | 30.081 | 44.723 | 55.024 | 1.00 29.32 | AAAA |
| ATOM | 2399 | CD1 | LEU | A 302 | | 30.119 | 44.840 | 53.502 | 1.00 27.38 | AAAA |
| ATOM | 2400 | CD2 | LEU | A 302 | | 31.296 | 45.389 | 55.613 | 1.00 27.36 | AAAA |
| ATOM | 2401 | C | LEU | A 302 | | 29.398 | 46.187 | 57.764 | 1.00 26.41 | AAAA |
| | 2402 | ō | | A 302 | | 29.874 | 45.648 | 58.755 | 1.00 26.62 | |
| ATOM | 2403 | N | AT.A | A 303 | | 29.756 | 47.397 | 57.353 | 1.00 26.50 | AAAA |
| ATOM | 2403 | CA | AT.A | A 303 | | 30.778 | 48.176 | 58.022 | 1.00 25.92 | AAAA |
| ATOM | | CB | 312 | A 303 | | 31.001 | 49.475 | 57.277 | 1.00 25.24 | AAAA |
| ATOM | 2405 | | | A 303 | | 30.490 | 48.464 | 59.487 | 1.00 26.03 | AAAA |
| MOTA | 2406 | Ç. | אנה | A 303 | | 31.325 | 48.175 | 60.340 | 1.00 26.95 | AAAA |
| MOTA | 2407 | 0 | ALA. | A 304 | | 29.322 | 49.028 | 59.792 | 1.00 25.29 | AAAA |
| MOTA | 2408. | N | ARG | A 304 | | 28.999 | 49.353 | 61.179 | 1.00 23.46 | AAAA |
| MOTA | 2409 | CA | ARG | A 304 | | 27.641 | 50.059 | 61.291 | 1.00 23.78 | AAAA |
| MOTA | 2410 | CB | AKG | A 304 | • | 27.553 | 51.451 | 60.629 | 1.00 24.59 | AAAA |
| MOTA | 2411 | CG | ARG | A 304 | | 26.302 | 52.223 | 61.091 | 1.00 25.85 | AAAA |
| MOTA | 2412 | CD | ARG | A 304 | | 25.067 | 51.465 | 60.869 | 1.00 27.54 | AAAA |
| MOTA | 2413 | NE | ARG | A 304 | | 23.007 | 51.547 | 61.637 | 1.00 28.36 | AAAA |
| ATOM | 2414 | CZ | ARG | A 304 | | | 52.362 | 62.695 | 1.00 26.48 | AAAA |
| ATOM | 2415 | NH1 | ARG | A 304 | | 23.957 | 50.794 | 61.358 | 1.00 28.45 | AAAA |
| ATOM | 2416 | NH2 | ARG | A 304 | | 22.910 | 48.118 | 62.053 | 1.00 23.18 | AAAA |
| ATOM | 2417 | С | ARG | A 304 | | 28.991 | | 63.135 | 1.00 22.26 | AAAA |
| ATOM | 2418 | 0 | ARG | A 304 | | 29.591 | 48.099 | 61.560 | 1.00 23.20 | AAAA |
| MOTA | 2419 | N | | A 305 | | 28.330 | 47.075 | | 1.00 22.33 | AAAA |
| ATOM | 2420 | CA | | A 305 | | 28.200 | 45.817 | 62.292 61.516 | 1.00 22.17 | AAAA. |
| ATOM | 2421 | CB | ALA | A 305 | | 27.319 | 44.866 | | | AAAA |
| ATOM | 2422 | С | ALA | A 305 | | 29.516 | 45.137 | 62.621 | | AAAA |
| ATOM | 2423 | 0 | ALA | A 305 | | 29.763 | 44.757 | 63.760 | | AAAA |
| MOTA | 2424 | N | TRP | A 306 | | 30.366 | 44.969 | 61.620 | | AAAA |
| MOTA | 2425 | CA | TRP | A 306 | | 31.634 | | 61.861 | | AAAA |
| | 2426 | CB | | A 306 | | 32.279 | 43.885 | 60.553 | | AAAA |
| ATOM | 2427 | CG | TRP | A 306 | | 31.703 | 42.618 | 60.004 | | |
| MOTA | | CD. | ממד כ | A 306 | | 31.886 | 42.103 | 58.683 | 1.00 19.54 | AAAA |
| ATOM | 2428 | CD | ממת כ | A 306 | | 31.352 | 40.795 | 58.668 | | AAAA |
| MOTA | 2429 | CE | O INF | A 306 | | 32.456 | 42.616 | 57.510 | 1.00 19.59 | AAAA |
| ATOM | 2430 | CE. |) IRP | A 300 | | 31.071 | | | 1.00 20.51 | AAAA |
| MOTA | 2431 | | 1 TKP | A 306 | | 30.864 | 40.537 | | 1.00 19.74 | AAAA |
| MOTA | 2432 | | 1 TRP | A 306 | | 31.368 | 39.990 | | | AAAA |
| MOTA | 2433 | CZ: | 2 TRP | A 306 | | | | | | AAAA |
| MOTA | 2434 | | 3. TRP | A 306 | | 32.474 | 41.810 40.513 | | 45 64 | AAAA |
| ATOM | 2435 | CH | 2 TRP | A 306 | | 31.933 | | | | AAAA |
| ATOM | 2436 | | TRP | A 306 | | 32.571 | | | | AAAA |
| ATOM | 2437 | | TRP | A 306 | | 33.459 | | | 10 | AAAA |
| ATOM | 2438 | | THR | A 307 | | 32.373 | | | | AAAA |
| ATOM | 2439 | | THR | A 307 | | 33.175 | 47.399 | | | AAAA |
| | 2440 | | THR | A 307 | | 32.861 | | | | AAAA |
| ATOM | 2441 | | 1 THR | A 307 | | 33.329 | 49.159 | 61.718 | | AAAA |
| MOTA | | | 7 THE | A 307 | | 33.523 | | 64.030 | 1.00 20.09 | AAAA |
| MOTA | . 2442 | | _ IND | | | | | - | | • |
| | | | | | | | | | | |

| - | | | | | | | | | | | | |
|--------------|--------------|-----|-------|---------|-------|--------|------------------|------------------|------|------|--------------|--------------|
| - 501 | 2442 | С | THR | Δ | 307 | 32.853 | 47.135 | 64.893 | 1.00 | | | AAAA |
| ATOM | 2443 | 0 | THR | Δ | 307 | 33.738 | 47.175 | 65.747 | 1.00 | | | AAAA |
| ATOM | 2444 2445 | Ŋ | LEU | Δ | 308 | 31.588 | 46.851 | 65.192 | 1.00 | | | AAAA |
| MOTA | _ | | LEU | | | 31.189 | 46.543 | 66.559 | 1.00 | 21 | .10 | AAAA |
| MOTA | 2446 | | LEU | | | 29.671 | 46.340 | 66.644 | 1.00 | | | AAAA |
| ATOM | 2447 | CB | LEU | Α | 308 | 28.897 | 47.656 | 66.674 | 1.00 | | | AAAA |
| MOTA | 2448 | | LEU | | | 27.397 | 47.473 | 66.411 | 1.00 | 19 | .91 | AAAA |
| ATOM | 2449 | | LEU | | | 29.177 | 48.283 | 68.045 | 1.00 | 21 | .04 | AAAA |
| MOTA | 2450 | | LEU | | | 31.886 | 45.284 | 67.052 | 1.00 | 21 | .98 | AAAA |
| ATOM | 2451 | | LEU | 7 | 308 | 32.284 | 45.186 | 68.215 | 1.00 | 22 | .17 | AAAA |
| MOTA | 2452 | 0 | ILE | | | 32.023 | 44.310 | 66.165 | 1.00 | 22 | .32 | AAAA |
| MOTA | 2453 | N | ILE | ν. • | 309 | 32.658 | 43.069 | 66.544 | 1.00 | 23 | .12 | AAAA |
| MOTA | 2454 | CA | ILE | | | 32.590 | 42.016 | 65.413 | 1.00 | 22 | .33 | AAAA |
| ATOM | 2455 | CB | ILE | | | 33.356 | 40.787 | 65.827 | 1.00 | 21 | .76 | AAAA |
| MOTA | 2456 | CG2 | ILE | Α. | 309 | 31.140 | 41.678 | 65.061 | 1.00 | 22 | .16 | AAAA |
| MOTA | 2457 | CG1 | ILE | | | 30.366 | 41.037 | 66.166 | 1.00 | | | AAAA |
| ATOM | 2458 | CDI | TIF | Δ | 309 | 34.115 | 43.377 | 66.790 | 1.00 | | | AAAA |
| MOTA | 2459 | 0 | ILE | Δ | 309 | 34.734 | 42.828 | 67.709 | 1.00 | | | AAAA |
| MOTA | 2460 2461 | И | | | 310 | 34.673 | 44.253 | 65.957 | 1.00 | 24 | .70 | AAAA |
| MOTA | 2462 | CA | | | 310 | 36.075 | 44.570 | 66.099 | 1.00 | 24 | .20 | AAAA |
| ATOM | 2462 | CB. | TRP | | | 36.587 | 45.417 | 64.944 | 1.00 | | | AAAA |
| MOTA | 2464 | CG. | | | 310 | 38.040 | 45.712 | 65.123 | 1.00 | | | AAAA |
| MOTA | 2465 | CDS | TRP | A | 310 | 39.104 | 44.752 | 65.257 | 1.00 | | | AAAA |
| ATOM | 2465 | CE2 | TRP | A | 310 | 40.291 | 45.472 | 65.490 | 1.00 | | | AAAA |
| ATOM | 2467 | CE3 | TRP | A | 310 | 39.165 | 43.354 | 65.202 | | | 0.01 | AAAA |
| MOTA | 2468 | CD1 | | | 310 | 38.614 | 46.938 | 65.273 | | | 2.82 | AAAA |
| ATOM | 2469 | NE1 | | | 310 | 39.967 | 46.803 | 65.497 | | | 2.30 | AAAA |
| MOTA | 2470 | CZ2 | | | 310 | 41.521 | 44.845 | 65.668 | | | 9.91 | AAAA |
| MOTA | 2471 | CZ3 | | | 310 | 40.388 | 42.734 | 65.381 | 1.00 |) 19 | 80.6 | AAAA |
| MOTA | 2472 | CH2 | | | 310 | 41.547 | 43.477 | 65.610 | 1.00 |) 19 | 9.40 | AAAA |
| MOTA MOTA | 2473 | C | | | 310 | 36.318 | 45.279 | 67.411 | 1.0 | 2: | 5.26 | AAAA |
| MOTA | 2474 | Ö | | | 310 | 37.262 | 44.945 | 68.109 | 1.00 | 2 | 4.71 | AAAA |
| ATOM | 2475 | N | | | 311 | 35.467 | 46.247. | | 1.0 | 0 20 | 6.76 | AAAA AAAA |
| MOTA | 2476 | CA | | | 311 | 35.608 | 46.975 | 69.007 | 1.0 | 0 2 | 7.89 | AAAA |
| MOTA | 2477 | CB | CYS | Α | 311 | 34.548 | 48.081 | 69.113 | 1.0 | 0 2 | 8.98 | AAAA |
| MOTA | 2478 | SG | | | 311 | 34.798 | 49.462 | 67.991 | 1.0 | 0 3 | 1.89 | AAAA |
| ATOM | 2479 | С | CYS | A | 311 | 35.495 | 46.043 | 70.212 | 1.0 | 0 2 | 7.51 6.90 | AAAA |
| ATOM | 2480 | 0 | CYS | Α | 311 | 36.289 | 46.127 | 71.135 | 1.0 | 0 2 | 7.33 | AAAA |
| ATOM | 2481 | N | | | 312 | 34.495 | 45.169 | 70.187 | 1.0 | 0 2 | 8.03 | AAAA |
| ATOM | 2482 | CA | | | 312 | 34.246 | 44.210 | 71.250 | 1.0 | 0 2 | 8.55 | AAAA |
| ATOM | 2483 | CB | | | 312 | 33.106 | 43.287 | 70.850 | | | 8.93 | AAAA |
| ATOM | 2484 | CG | GLU | Α | 312 | 31.903 | 43.333 | 71.741 | 1.0 | 0 2 | 9.78 | AAAA |
| MOTA | 2485 | CD | GLU | Α | 312 | 32.232 | 42.958 | 73.154 73.345 | | ก็จ | 0.81 | AAAA |
| MOTA | 2486 | 0El | GLU | A | 312 | 32.954 | 41.957 | 74.071 | | กร | 0.79 | AAAA |
| ATOM | 2487 | OE2 | GLU | A | 312 | 31.754 | 43.653 | 71 514 | | 0 2 | 8.91 | AAAA |
| MOTA | 2488 | С | GLU | A | 312 | 35.463 | 43.357 | 72 662 | 1 0 | 0 3 | 0.57 | AAAA |
| ATOM | 2489 | 0 | | | 312 | 35.822 | 43.110 | 70.436 | | 0 2 | 9.04 | AAAA |
| MOTA | 2490 | N | | | 313 | 36.081 | 42.889 42.045 | 70.516 | | 0 2 | 8.87 | AAAA |
| ATOM | 2491 | CA | LEU | - 2 | 313 | 37.266 | 41.373 | 69.157 | | 0 2 | 9.39 | AAAA |
| MOTA | 2492 | CB | | | 313 | 37.524 | 40.311 | 68.644 | | 0 3 | 0.32 | AAAA |
| ATOM | 2493 | CG | | | 313 | 36.548 | 39.872 | 67.215 | | 0 3 | 0.26 | AAAA |
| ATOM | 2494 | CD1 | . LEU | 7.7 | 313 | 36.910 | 39.114 | 69.593 | _ | 0 3 | 0.42 | AAAA |
| ATOM | 2495 | | | | 313 | 36.582 | 42.888 | | _ | 0 2 | 7.75 | AAAA |
| MOTA | 2496 | С | | | 313 | 38.474 | 42.553 | | | 0 2 | 7.34 | AAAA |
| ATOM | 2497 | 0 | | | 313 | 39.215 | | | | 0 2 | 7.95 | AAAA |
| MOTA | 2498 | N | SEF | | 314 | 38.642 | | 70.376 | | 0 2 | 8.62 | AAAA |
| MOTA | 2499 | | | | 314 | 39.736 | | | | 0 2 | 7.49 | AAAA |
| ATOM | 2500 | | | | 314 | 39.690 | | | | 0 3 | 0.12 | AAAA |
| ATOM | 2501 | | | | A 314 | 40.703 | | | | 0 2 | 9.67 | AAAA |
| ATOM | 2502 | | | | A 314 | 39.666 | | | | 0 2 | 9.00 | AAAA |
| ATOM | 2503 | | SEF | 2 | A 314 | 40.488 | | · | _ | 00 | 30.78 | AAAA |
| MOTA | 2504 | | GL' | () | A 315 | 38.676 | | | _ | 00 3 | 32.92 | AAAA |
| MOTA | 2505 | | GL | 7 | A 315 | 38.535 | | | | 00 | 34.92 | AAAA |
| ATOM | 2506 | | GL | Y . | A 315 | 38.542 | | | | 00 | 35.17 | AAAA |
| ATCM | 2507 | | | | A 315 | 39.142 | | | | 00 | 36.88 | AAAA |
| MOTA | 2508 | N | AR | 3 . | A 316 | 37.881 | 10.041 | | | | | • |
| .* | • | | • | | | | | | | | | |

| ATOM | 2509 | CA | ARG | Α | 316 | 3. | 7.841 | 49.493 | 72.702 | 1.00 39.49 | AAAA |
|------|-------|-------|-------|------------|-----|-----|-------|---------|----------|------------|--------|
| | 2510 | CB | ARG | Δ | 316 | 31 | 8.608 | 49.968 | 71.484 | 1.00 39.86 | AAAA |
| ATOM | | | | | | | 7.946 | 49.677 | 70.161 | 1.00 40.77 | AAAA |
| MOTA | 2511 | CG | ARG | | | | | | | 1.00 41.47 | AAAA |
| MOTA | 2512 | CD | ARG | A | 316 | | 8.843 | 50.226 | 69.077 | | |
| MOTA | 2513 | NE | ARG | Α | 316 | 4 | 0.140 | 49.566 | 69.092 | 1.00 42.36 | AAAA |
| | 2514 | CZ | ARG | | | 4 | 1.224 | 50.057 | 68.515 | 1.00 43.38 | AAAA |
| ATOM | | | | | | | 1.159 | 51.217 | 67.882 | 1.00 44.76 | AAAA |
| MOTA | 2515 | NHl | | | | | | | | 1.00 43.71 | AAAA |
| MOTA | 2516 | NH2 | ARG | Α | 316 | | 2.361 | 49.385 | 68.556 | | |
| | 2517 | C | ARG | A | 316 | 3 | 6.418 | 50.015 | 72.631 | 1.00 41.54 | AAAA |
| ATOM | | | ARG | | | | 5.564 | 49.429 | 71.959 | 1.00 42.64 | AAAA |
| MOTA | 2518 | 0 | | | | | | 51.119 | 73.329 | 1.00 43.10 | AAAA |
| ATOM | 2519 | N | GLU | | | | 6.163 | | | | AAAA |
| MOTA | 2520 | CA | GLU | Α | 317 | 3. | 4.830 | 51.720 | 73.356 | 1.00 44.51 | |
| | 2521 | CB | GLU | | | 3 | 4.809 | 52.936 | 74.293 | 1.00 46.17 | AAAA |
| MOTA | | | | | 317 | 3 | 4.472 | 52.614 | 75.759 | 1.00 49.65 | AAAA |
| ATOM | 2522 | CG | | | | | 5.426 | 51.623 | 76.439 | 1.00 52.51 | AAAA |
| MOTA | 2523 | CD | | | 317 | | | | | 1.00 53.37 | AAAA |
| MOTA | 2524 | | GLU | | | | 5.153 | 51.251 | 77.607 | | |
| ATOM | 2525 | OE2 | GLU | Α | 317 | 3 | 6.444 | 51.214 | 75.831 | 1.00 54.14 | AAAA |
| | 2526 | C | | | 317 | 3 | 4.318 | 52.098 | 71.974 | 1.00 43.86 | AAAA |
| ATOM | | | | | | | 5.067 | 52.532 | 71.108 | 1.00 42.46 | AAAA |
| MOTA | 2527 | Ο, | | | 317 | | | | 71.779 | 1.00 44.79 | AAAA |
| ATOM | 2528 | N | VAL | Α | 318 | | 3.023 | 51.916 | | | AAAA |
| ATOM | 2529 | CA | VAL | Α | 318 | 3 | 2.394 | 52.197 | 70.502 | 1.00 45.57 | |
| | 2530 | CB | MAT. | Δ | 318 | 3 | 1.098 | 51.369 | 70.324 | 1.00 45.36 | AAAA |
| ATCM | | | | | | | 0.537 | 51.558 | 68.924 | 1.00 45.44 | AAAA |
| ATOM | 2531 | | VAL | | | | | | 70.612 | 1.00 46.35 | AAAA |
| MOTA | 2532 | CG2 | VAL | | | | 1.366 | 49.911 | | | AAAA |
| MOTA | 2533 | С | VAL | Α | 318 | 3 | 2.007 | 53.652 | 70.377 | 1.00 46.41 | |
| | 2534 | 0 | | | 318 | 3 | 1.199 | 54.145 | 71.165 | 1.00 46.53 | AAAA |
| MOTA | | | DBO | ~ | 319 | | 2.584 | 54.370 | 69.396 | 1.00 46.89 | AAAA . |
| MOTA | 2535 | N | | | | | 3.581 | 54.017 | 68.375 | 1.00 46.44 | AAAA |
| MOTA | 2536 | CD | | | 319 | | | | | 1.00 47.62 | AAAA |
| ATOM | 2537 | CA | | | 319 | | 2.209 | 55.774 | 69.247 | | |
| ATOM | 2538 | CB | PRO | Α | 319 | 3 | 3.022 | 56.206 | 68.024 | 1.00 46.96 | AAAA |
| | | CG | DDO | Δ | 319 | | 3.161 | 54.922 | 67.251 | 1.00 46.38 | AAAA |
| MOTA | 2539 | _ | | | | | 0.709 | 55.743 | 68.977 | 1.00 48.64 | AAAA |
| MOTA | 2540 | С | | | 319 | | | | | 1.00 48.61 | AAAA |
| MOTA | 2541 | 0 | PRO | Α | 319 | | 0.236 | 54.860 | 68.262 | | AAAA |
| ATOM | 2542 | N | GLU | A | 320 | | 9.944 | 56:.667 | 69.544 | 1.00 49.24 | |
| | 2543 | CA | | | 320 | 2 | 8.522 | .56.598 | 69.288 | 1.00 50.01 | AAAA |
| ATOM | | | | | 320 | | 7.720 | 57.330 | 70.363 | 1.00 51.15 | AAAA |
| MOTA | 2544 | CB | | | | | | | 70.339 | 1.00 53.01 | AAAA |
| ATOM | 2545 | CG | | | 320 | | 7.828 | 58.831 | | | AAAA |
| MOTA | 2546 | CD | GLU | Α | 320 | 2 | 6.825 | 59.474 | 71.282 | 1.00 54.34 | |
| ATOM | 2547 | OFI | GLU. | Α | 320 | 2 | 5.604 | 59.273 | 71.077 | 1.00 54.04 | AAAA |
| | | | | | 320 | 2 | 7.255 | 60.171 | 72.228 | 1.00 55.06 | AAAA |
| atom | 2548 | | GLU | ~ | 220 | | 8.206 | 57.168 | 67.921 | 1.00 49.78 | AAAA |
| ATOM | 2549 | С | | | 320 | | | | | 1.00 49.79 | AAAA |
| MOTA | 2550 | O | | | 320 | _ | 7.170 | 56.861 | 67.324 | | AAAA |
| ATOM | 2551 | N | LYS | A | 321 | . 2 | 9.116 | 57.980 | 67.407 | 1.00 49.26 | |
| | 2552 | CA | | | 321 | 2 | 8.906 | 58.589 | 66.109 | 1.00 49.20 | AAAA |
| ATOM | | | 1370 | , | 221 | | 8.873 | 60.106 | 66.251 | 1.00 50.38 | AAAA |
| MOTA | 2553 | CB | | | 321 | | | | | 1.00 52.88 | AAAA |
| MOTA | : 354 | CG | LYS | Α | 321 | - | 0.234 | 60.674 | 66.634 | | AAAA |
| ATOM | :.555 | CD | LYS | A | 321 | 3 | 0.717 | 60.180 | 68.002 | 1.00 53.76 | |
| | 2356 | CE | LVS | Δ | 321 | 3 | 2.229 | 60.348 | 68.154 | 1.00 55.00 | AAAA |
| ATOM | | | 1 7 0 | `` | 321 | | 2.715 | 61.725 | 67.829 | 1.00 55.95 | AAAA |
| ATOM | 2557 | ΝZ | | | | | | 58.207 | 65.171 | 1.00 48.64 | AAAA |
| ATOM | 2558 | С | | | 321 | | 0.037 | | | | AAAA |
| ATOM | 2559 | 0 | LYS | A | 321 | | 1.052 | 57.650 | 65.590 | 1.00 48.58 | |
| | 2560 | N | | | 322 | 2 | 9.854 | 58.511 | 63.894 | 1.00 47.78 | AAAA |
| ATOM | | | | | | | 0.870 | 58.238 | 62.896 | 1.00 46.13 | AAAA |
| MOTA | 2561 | CA | ייביי | A | 322 | | | | 61.638 | 1.00 46.84 | AAAA |
| ATOM | 2562 | CB | LEU | A | 322 | | 0.248 | 57.638 | | 1.00 40.04 | AAAA |
| ATOM | 2563 | CG | LEU | A | 322 | 2 | 9.240 | 56.504 | 61.848 | 1.00 47.71 | |
| | | CD1 | T.FII | 2 | 322 | | 8.788 | 55.998 | 60.491 | 1.00 48.02 | AAAA |
| MOTA | 2564 | CDI | 7 577 | - | 322 | | 9.853 | 55.374 | 62.667 | 1.00 48.21 | AAAA |
| MOTA | 2565 | | | | 322 | | | | 62.580 | 1.00 44.61 | AAAA |
| ATOM | 2566 | С | | | 322 | | 1.427 | 59.608 | | 1 00 44 72 | AAAA |
| MOTA | 2567 | 0 | LEU | A | 322 | 3 | 0.674 | 60.571 | 62.491 | 1.00 44.73 | |
| | 2568 | N | | | 323 | | 2.741 | 59.706 | 62.447 | 1.00 42.66 | AAAA |
| ATOM | | | | | 323 | | 3.360 | 60.976 | 62.135 | 1.00 41.19 | AAAA |
| ATOM | 2569 | CA | NCA | - ^ | 223 | | | | 62.402 | 1.00 41.07 | AAAA |
| ATOM | 2570 | CB | | | 323 | | 4.860 | | | | AAAA |
| ATOM | 2571 | CG | ASN | A | 323 | | 5.576 | 60.001 | 61.436 | | |
| | 2572 | | ASN | A 1 | 323 | 3 | 5.117 | 58.901 | 61.147 | 1.00 42.46 | AAAA |
| ATOM | | VID.3 | 3 CM | | 323 | | 6.720 | | 60.943 | 1.00 41.77 | AAAA |
| atom | 2573 | | VOW | | 222 | | | | | | AAAA |
| ATOM | 2574 | С | ASN | ı A | 323 | - | 3.068 | 61.223 | _ 55.556 | | |
| • | | • | | | | | | | | | |

| | • | | | | 0- | | | | • | |
|--------------|--------------|----------|----------------|----------------|----|------------------|------------------|------------------|--------------------------|--------------|
| | | _ | | 222 | • | 32.430 | 60.395 | 60.010 | 1.00 40.19 | aaaa |
| MOTA | 2575 | 0 . 4 | ASN A ASN A | 324 | | 33.523 | 62.352 | 60.129 | 1.00 40.11 | aaaa |
| ATOM | 2576 | | ASN A ASN A | | | 33.268 | 62.699 | 58.735 | 1.00 39.99 | AAAA |
| MOTA | 2577 | | ASN A ASN A | | | 33.711 | 54.128 | 58.472 | 1.00 39.54 | AAAA |
| MOTA | 2578 | | ASN A | | | 33.003 | 65.114 | 59.361 | 1.00 40.88 | AAAA |
| MOTA | 2579 | CG . | ASN A | 324 | | 31.763 | 65.145 | 59.417 | 1.00 40.77 | AAAA |
| MOTA | 2580 | MD3 | ASN A | 324 | | 33.779 | 65.938 | 60.064 | 1.00 40.63 | AAAA |
| ATOM | 2581 2582 | C | ASN A | 324 | | 33.918 | 61.786 | 57.712 | 1.00 40.10 | AAAA |
| ATOM | 2583 | | ASN A | | | 33.320 | 61.468 | 56.678 | 1.00 39.24 | AAAA |
| MOTA | 2584 | | LYS A | | | 35.144 | 61.376 | 58.011 | 1.00 40.41 | AAAA |
| MOTA MOTA | 2585 | CA | LYS A | 325 | | 35.908 | 60.519 | 57.126 | 1.00 41.41 | AAAA |
| MOTA | 2586 | | LYS A | | | 37.262 | 60.201 | 57.761 | 1.00 42.64 | aaaa aaaa |
| ATOM | 2587 | CG | LYS A | 325 | | 38.224 | 59.504 | 56.828 | 1.00 44.45 1.00 45.61 | AAAA |
| ATOM | 2588 | CD | LYS A | 325 | | 39.575 | 59.199 | 57.491 | 1.00 45.88 | AAAA |
| ATOM | 2589 | CE | LYS A | 325 | | 40.358 | 60.464 | 57.850 58.404 | 1.00 45.88 | AAAA |
| ATOM | 2590 | NZ | LYS ? | A 325 | | 41.717 | 60.151 | 56.856 | 1.00 41.56 | AAAA |
| ATOM | 2591 | С | LYS A | A 325 | | 35.124 | 59.248 58.781 | 55.716 | 1.00 41.35 | AAAA |
| MOTA. | 2592 | | | A 325 | | 35.042 34.524 | 58.703 | 57.906 | 1.00 41.32 | AAAA |
| MOTA | 2593 | N | | 326 | | 33.732 | 57.492 | 57.774 | 1.00 41.07 | AAAA |
| MOTA | 2594 | CA | ALA A | A 326 | | 33.452 | 56.912 | 59.143 | 1.00 40.87 | AAAA |
| MOTA | 2595 | | ALA : | A 326 A 326 | | 32.420 | 57.722 | 57.019 | 1.00 41.24 | AAAA |
| MOTA | 2596 | C | ALA A | A 326 | | 32.045 | 56.913 | 56.174 | 1.00 40.91 | AAAA |
| ATOM | 2597 | И | | A 327 | | 31.719 | 58.815 | 57.316 | 1.00 41.92 | AAAA |
| MOTA | 2598 2599 | CA | | A 327 | | 30.451 | 59.097 | 56.631 | 1.00 42.20 | AAAA |
| MOTA MOTA | 2600 | CB | | A 327 | | 29.796 | 60.374 | 57.170 | 1.00 43.61 | AAAA AAAA |
| ATOM | 2601 | CG | | A 327 | | 29.534 | 60.413 | 58,670 | 1.00 45.83 | AAAA |
| ATOM | 2602 | CD | LYS 2 | A 327 | .* | 28.745 | 61.681 | 59.029 | 1.00 47.34 1.00 48.28 | AAAA |
| ATOM | 2603 | CE | LYS | A 327 | | 28.682 | 61.952 | 60.538 | 1.00 48.28 | AAAA |
| ATOM | 2604 | NZ | LYS . | A 327 | | 28.090 | 60.845 | 61.351 55.125 | 1.00 41.33 | AAAA |
| ATOM | 2605 | С | | A 327 | | 30.673 | 59.266 | 54.309 | 1.00 40.78 | AAAA |
| MOTA | 2606 | 0 | | A 327 | | 29.879 31.761 | 58.797 59.950 | 54.781 | 1.00 40.39 | AAAA |
| ATOM | 2607 | Ŋ | | A 328 | | 32.129 | 60.217 | 53.399 | 1.00 38.91 | aaaa |
| MOTA | 2608 | CA | GLU . | A 328 A 328 | | 33.300 | 61.199 | 53.369 | 1.00 40.04 | AAAA |
| MOTA | 2609 | CB | GLU . | A 328 | | 32.941 | 62.576 | 53.909 | 1.00 41.94 | AAAA |
| MOTA | 2610 2611 | CG CD | | A 328 | | 34.131 | 63.515 | 53.994 | 1.00 43.77 | AAAA |
| ATOM ATOM | 2612 | | | A 328 | | 34.904 | 63.595 | 53.010 | 1.00 44.29 | 4444 4444 |
| ATOM | 2613 | OE2 | GLU | A 328 | | 34.285 | 64.189 | 55.040 | 1.00 45.11 | AAAA |
| ATOM | 2614 | C | GLU | A 328 | | 32.497 | 58.938 | 52.675 | 1.00 37.39 1.00 37.31 | AAAA |
| MOTA | 2615 | 0 | | A 328 | | 32.114 | 58.722 | 51.525 53.355 | 1.00 37.31 | AAAA |
| ATOM | 2616 | N | | A 329 | | 33.255 | 58.091 56.820 | 52.783 | 1.00 33.03 | AAAA |
| ATOM | 2617 | CA | | A 329 | | 33.657 | 56.012 | 53.813 | 1.00 30.62 | AAAA |
| MOTA | 2618 | CB | | A 329 | | 34.451 34.760 | | 53.481 | 1.00 27.48 | AAAA |
| MOTA | 2619 | CG | LEU | A 329 | | 35.549 | 54.453 | 52.193 | 1.00 ?6.24 | AAAA |
| MOTA | 2620 | CDI | LEU | A 329 A 329 | | 35.514 | 53.936 | 54.622 | 1.00 25.74 | AAAA |
| MOTA | | | LEU | A 329 | | 32.405 | 56.057 | | 1.00 33.24 | AAAA |
| MOTA | 2622 2623 | c o | | A 329 | | 32.239 | 55.708 | | 1.00 32.72 | AAAA |
| ATOM | 2624 | N | | A 330 | | 31.519 | 55.810 | | 1.00 33.92 | AAAA AAAA |
| MOTA MOTA | 2625 | CA | LEU | A 330 | | 30.289 | 55.090 | | 1.00 34.91 | AAAA |
| ATOM | 2626 | CB | | A 330 | | 29.411 | 55.023 | | 1.00 34.02 | AAAA |
| MOTA | 2627 | CG | LEU | A 330 | | 30.067 | 54.236 | | 1.00 34.06 1.00 33.63 | AAAA |
| ATOM | . 2623 | CD1 | LEU | A 330 | | 29.096 | | | | AAAA |
| ATOM | 2629 | CD2 | LEU | A 330 | | 30.512 | . . | | | AAAA |
| MOTA | 2630 | | | A 330 | | 29.499 | | | | AAAA |
| ATOM | 2631 | 0 | | A 330 | | 28.984 29.415 | | | | AAAA |
| MOTA | 2632 | | LYS | A 331 | | 29.415 | | | 1.00 41.05 | AAAA |
| MOTA | 2633 | | | A 331 | | 28.407 | | | 1.00 41.83 | AAAA |
| MOTA | 2634 | | | A 331 A 331 | | 27.584 | | | 1.00 43.26 | AAAA |
| MOTA | 2635 | | TVC | A 331 | | 27.202 | | | 1.00 44.15 | AAAA |
| ATOM | 2636 | | | A 331 | | 26.182 | 61.333 | 51,730 | 1.00 45.71 | <i>አ</i> ሕሕሕ |
| ATOM | 2637 2638 | | | A 331 | | 25.695 | 62.735 | 51.993 | | АААА АААА |
| ATOM | 2639 | | | A 331 | | 29.342 | 57.681 | 49.490 | 1.00 42 22 | AAAA |
| MOTA MOTA | 2640 | | | A 331 | | 28.712 | 57.980 | 48.480 | 1.00 41.94 | , where |
| W 1 (1) | | | | | | | | | | |

| | | | | | _ | | | | | | |
|--------------|--------------|--------|--------|-------|----|------------------|------------------|------------------|------|--------------------|--------------|
| | | | SER A | 222 | 30 | .618 | 57.316 | 49.463 | 1.00 | 44.45 | AAAA |
| MOTA | 2641 | | SER A | 332 | | .351 | 57.271 | 48.202 | | 46.88 | AAAA |
| MOTA | 2642 | | SER A | | | .854 | 57.416 | 48.435 | 1.00 | 46.49 | AAAA |
| MOTA | 2643 | | SER A | | | .380 | 56.263 | 49.058 | 1.00 | 45.65 | AAAA |
| ATOM | 2644 | | SER A | | | .093 | 55.959 | 47.494 | 1.00 | 48.73 | AAAA |
| MOTA | 2645 | C | SER A | 332 | | .262 | 55.854 | 46.281 | 1.00 | 49.51 | AAAA |
| ATOM - | 2646 | 0 | ILE A | 332 | | .697 | 54.952 | 48.258 | 1.00 | 50.62 | AAAA |
| MOTA | 2647 | | ILE A | | | .420 | 53.648 | 47.686 | 1.00 | 52.65 | AAAA |
| MOTA | 2648 | CA | ILE A. | 333 | | .246 | 52.584 | 48.779 | 1.00 | 52.35 | AAAA |
| ATOM | 2649 | CB | ILE A | 333 | | .889 | 51.248 | 48.157 | 1.00 | 51.40 | AAAA |
| ATOM | 2650 | CG1 | ILE A | 333 | 31 | .522 | 52.465 | 49.596 | 1.00 | 52.29 | AAAA |
| MOTA | 2651 2652 | CD1 | ILE A | 333 | | .403 | 51.463 | 50.696 | 1.00 | 53.23 | AAAA AAAA |
| MOTA | 2653 | C | ILE A | 333 - | 29 | .120 | 53.712 | 46.924- | 1.00 | 54.42 | AAAA |
| MOTA | 2654 | 0 | ILE A | 333 | | .122 | 54.178 | 47.462 | 1.00 | 55.10 | AAAA |
| MOTA | 2655 | N | ASP A | 334 | | .118 | 53.274 | 45.672 | 1.00 | 56.56 | . AAAA |
| MOTA ATOM | 2656 | CA | ASP A | 334 | | .863 | 53.263 | 44.940 | 1.00 | 59.13 59.64 | AAAA |
| ATOM | 2657 | СВ | ASP A | 334 | | 3.050 | 53.460 | 43.433 | 1.00 | 59.23 | AAAA |
| ATOM | 2658 | CG | ASP A | 334 . | | 3.976 | 52.446 | 42.823 | 1.00 | 58.87 | AAAA |
| ATOM | 2659 | OD1 | ASP A | 334 | | 3.853 | 52.194 | 41.606 | 1.00 | 59.34 | AAAA |
| ATOM | 2660 | OD2 | ASP A | 334 | | 839 | 51.925 | 43.559 45.215 | 1 00 | 60.95 | AAAA |
| ATOM | 2661 | С | ASP A | 334 | | 7.251 | 51.898 | 44.840 | 1 00 | 61.15 | AAAA |
| MOTA | 2662 | 0 | ASP A | 334 | | 7.803 | 50.861 | 45.897 | 1 00 | 62.56 | AAAA |
| ATOM | 2663 | N | PHE A | 335 | | 5.113 | 51.914 50.701 | 46.257 | 1.00 | 64.12 | AAAA |
| ATOM | 2664 | CA | PHE A | | | 5.414 | 50.701 | 47.779 | 1.00 | 64.40 | AAAA |
| MOTA | 2665 | CB | PHE A | | | 5.311 | 49.714 | 48.263 | 1.00 | 64.98 | AAAA |
| MOTA | 2666 | CG | PHE A | 335 | | 4.224 4.180 | 48.379 | 47.868 | 1.00 | 65.54 | AAAA |
| MOTA | 2667 | CD1 | PHE A | 335 | | 3.234 | 50.197 | 49.107 | 1.00 | 65.12 | AAAA |
| MOTA | 2668 | CD2 | PHE A | 333 | 2 | 3.163 | 47.539 | 48.305 | 1.00 | 65.75 | AAAA |
| MOTA | 2669 | CEI | PHE A | 333 | | 2.213 | 49.367 | 49.552 | 1.00 | 65.79 | AAAA |
| MOTA | 2670 | | PHE A | 335 | _ | 2.177 | 48.034 | 49.150 | 1.00 | 66.01 | AAAA |
| MOTA | 2671 | CZ | PHE A | 335 | | 4.025 | 50.626 | 45.640 | 1.00 | 65.41 | AAAA |
| MOTA | 2672 | C | PHE A | 335 | | 3.591 | 49.564 | 45.184 | 1.00 | 65.27 | AAAA |
| MOTA | 2673 2674 | 0 N | GLU A | | | 3.338 | 51.763 | 45.618 | 1.00 | 66.38 | AAAA AAAA |
| MOTA | 2675 | CA | GLU A | 336 | 2 | 1.980 | 51.826 | 45.097 | 1.00 | 67.49 | AAAA |
| MOTA | 2676 | CB | GLU A | 336 | | 1.893 | 51.260 | 43.673 | 1.00 | 68.25 | AAAA |
| ATOM ATOM | 2677 | CG | GLU A | 336 | | 0.459 | 51.230 | 43.116 | 1.00 | 69.15 | AAAA |
| ATOM | 2678 | CD | GLU A | 336 | | 0.334 | 50.465 | 41.804 | 1.00 | 69.57 | AAAA |
| ATOM | 2679 | OE1 | GLU A | 336 | _ | 0.710 | 49.271 | 41.784 | 1.00 | 69.10 | AAAA |
| MOTA | 2680 | OE2 | GLU A | 336 | | 9.851 | 51.051 50.999 | | 1.00 | 67.68 | AAAA |
| ATOM | 2681 | С | GLU A | 336 | | 1.098 | 49.776 | | 1.00 | 67.58 | AAAA |
| ATOM | 2682 | 0 | GLU À | 336 | | 1.216 | 51.679 | | 1.00 | 67.87 | AAAA |
| MOTA | 2683 | N | GLU A | 337 | | 0.227 9.317 | | | 1.00 | 0 68.66 | AAAA |
| MOTA | 2684 | CA | GLU A | 337 | | .9.517 .8.583 | 52.085 | 48.502 | 1.0 | 0 68.88 | AAAA |
| MOTA | 2685 | CB | GLU A | A 337 | | 8.279 | | | 1.0 | 0 68.12 | AAAA |
| MOTA | 2686 | | GLU | . 33/ | | 9.527 | | | 1.0 | 0 67.70 | AAAA |
| MOTA | 2687 | | GLU . | 337 | | 0.319 | | | 1.0 | 0 67.05 | AAAA |
| MOTA | 2688 | _ | CLU . | . 337 | 1 | 9.711 | 50.518 | | 1.0 | 0 67.79 | AAAA |
| MOTA | 2689 | | CIII 2 | A 337 |] | 8.322 | | 46.827 | | 0 69.28 | AAAA |
| MOTA | 2690 | | GEU A | A 337 | | 7.886 | | | _ | 0 69.50 | AAAA |
| ATOM | 2691 | | SHE 1 | A 338 | 1 | 17.966 | 49.012 | | | 0 69.55 | AAAA AAAA |
| MOTA | 2692 2693 | | OHE ? | A 338 | | 17.035 | 48.176 | | | 0 69 67. | AAAA |
| ATOM | 2694 | | PHE 2 | A 338 | : | 16.995 | 46.759 | | | 0 70.51 | AAAA |
| MOTA | 2695 | | PHE | A 338 | : | 16.225 | 45.789 | | | 0 71.57 | AAAA |
| MOTA | 2696 | | 1 PHE | A 338 | | 16.666 | | | _ | 0 72.04 | AAAA |
| MOTA MOTA | 2697 | | 2 PHE | A 338 | | 15.052 | | | | 0 71.69 0 72.23 | AAAA |
| | 2698 | | 1 PHE | A 338 | | 15.944 | | | | 0 71.93 | AAAA |
| MOTA MOTA | 2699 | | 2 PHE | A 338 | | 14.323 | | | | 0 72.11 | AAAA |
| MOTA | 2700 | | PHE | A 338 | | 14.770 | | | | 0 69.26 | AAAA |
| ATOM | | - | PHE | 338 A | | 15.63 | | | _ | 0 68.86 | AAAA |
| ATOM | | - | PHE | A 338 | | 15.07 | | 9 45.434 | | 0 69.35 | AAAA |
| ATOM | | _ | ASP | A 339 | | 15.05 | | | | 0 69.61 | AAAA |
| ATOM | | | ASP | A 339 | | 13.73 | | | | 0 69.48 | AAAA |
| · ATOM | | | ASP | A 339 | | 13.13 | | | | 0 69.72 | 'AAAA |
| MOTA | | | ASP | A 339 | | 11.81 | 9 50.23 | . 47.47 | · · | | • |
| 71011 | | | | | | | | | | | |

| | | | 220 | 11.813 | 51.462 | 49.058 | 1.00 69.39 | AAAA |
|--------------|---------|-----------|---------|------------------|------------------|------------------|------------------------|------------------|
| MOTA | 2707 OI | ol ASP A | 339 | | 49.618 | | 1.00 69.78 | AAAA |
| ATOM | *** | D2 ASP A | 339 | | 51.035 | 47.440 | 1.00 69.95 | AAAA |
| MOTA | 2709 C | ASP A | 339 | | 51.815 | 48.333 | 1.00 69.92 | AAAA |
| ATOM | 2710 0 | ASP A | 339 | 14.305 | 51.389 | | 1.00 70.23 | AAAA |
| MOTA | 2711 N | ASP A | 340 | 13.810 | 52.748 | 45.699 | 1.00 70.39 | AAAA |
| MOTA | 2712 C | A ASP A | 340 | 14.023 | 53.283 | 45.041 | 1.00 70.64 | AAAA |
| MOTA | 2713 C | B ASP A | 340 | 12.757 | 52.517 | 43.791 | 1.00 70.86 | AAAA |
| ATOM | 2714 C | G ASP A | 340 | 12.397 | 51.302 | 43.903 | 1.00 70.93 | AAAA |
| ATOM | 2715 0 | D1 ASP A | 340 | 12.126 | 53.125 | 42.699 | 1.00 70.89 | AAAA |
| ATOM | 2716 0 | D2 ASP A | 340 | 12.399 14.482 | 53.674 | 46.807 | 1.00 70.63 | AAAA |
| MOTA | 2717 C | ASP A | | 15.688 | 53.847 | 47.008 | 1.00 71.13 | AAAA |
| ATOM | 2718 O | ASP A | 340 | 13.543 | 54.259 | 47.544 | 1.00 69.95 | AAAA |
| MOTA | 2719 N | | 341 | 13.947 | 55.150 | 48.619 | 1.00 69.17 | |
| MOTA | 2720 C | | 341 | 13.547 | 56.613 | 48.266 | 1.00 70.83 | |
| MOTA | 2721 C | _ | 341 | 14.098 | 57.601 | 49.347 | 1.00 73.44 | AAAA |
| ATOM | | G GLU A | | 13.956 | 59.071 | 48.951 | 1.00 75.27 | AAAA |
| MOTA | | D GLU A | 341 | 12.825 | 59.518 | 48.646 | 1.00 76.21 | AAAA |
| ATOM | _ | E1 GLU A | 341 | 14.984 | 59.786 | 48.954 | 1.00 75.69 | AAAA |
| ATOM | | E2 GLU A | 341 | 13.367 | 54.819 | 49.983 | 1.00 67.09 | AAAA |
| MOTA | 2726 C | GLU A | | 12.233 | 55.176 | 50.297 | 1.00 66.57 | AAAA |
| MOTA | 2727 C | | | 14.158 | 54.114 | 50.785 | 1.00 64.87 | AAAA |
| MOTA | 2728 N | | 342 | 13.767 | 53.779 | 52.148 | 1.00 62.55 | AAAA |
| MOTA | | A VAL A | | 14.265 | 52.377 | 52.589 | 1.00 62.81 | |
| MOTA | | B VAL A | 344 | 14.042 | 52.193 | 54.081 | 1.00 62.56 | AAAA |
| MOTA | | G1 VAL A | 342 | 13.513 | 51.298 | 51.849 | 1.00 63.69 | AAAA |
| ATOM | _ | G2 VAL A | 342 | 14.483 | 54.822 | 52.982 | 1.00 59.94 | AAAA |
| MOTA | 2733 | | 342 | 14.022 | 55.215 | 54.054 | 1.00 59.9 | l AAAA |
| MOTA | | | 3 342 | 15.609 | 55.278 | 52.442 | 1.00 56.85 | 5 AAAA |
| MOTA | | | 343 | 16.457 | 56.266 | 53.085 | 1.00 54.0 | 1 AAAA |
| MOTA | | CA ASP A | 343 | 15.639 | 57.446 | 53.605 | 1.00 54.1 | AAAA 8 |
| MOTA | | CG ASP A | 343 | 16.505 | 58.511 | 54.241 | 1.00 53.9 | AAAA 6 |
| MOTA | 2739 | DD1 ASP A | | 15.947 | 59.485 | 54.785 | 1.00 54.5 | 9 AAAA |
| MOTA | 2740 | OD2 ASP A | A 343 . | 17.747 | 58.373 | 54.191 | 1.00 53.6 | 1 AAAA 2 AAAA |
| ATOM | | C ASP | A 343 | 17.186 | 55.609 | 54.242 | 1.00 51.9 | _ |
| MOTA | | O ASP | A 343 | 16.611 | 55.371 | 55.307 | 1.00 51.8 | |
| MOTA MOTA | | N ARG | A 344 | 18.458 | 55.306 | 54.029 | 1.00 48.8 1.00 45.5 | |
| MOTA | | CA ARG | A 344 | 19.240 | 54.676 | 55.069 | 1.00 43.3 | • |
| ATOM | | CB ARG | A 344 | 19.847 | 53.369 | 54.573 | 1.00 41.7 | • |
| ATOM | | CG ARG | A 344 | 18.847 | 52.289 | 54.220 | 1.00 38.9 | _ |
| ATOM | | CD ARG | A 344 | 17.953 | 51.955 | 55.385 | 1.00 36.7 | |
| ATOM | | NE ARG | A 344 | 17.139 | 50.781 | 55.096 55.888 | 1.00 34.8 | |
| ATOM | 2749 | CZ ARG | A 344 | 16.176 | 50.316 | 57.033 | 1.00 34.1 | |
| MOTA | 2750 | NH1 ARG | A 344 | 15.890 | 50.927 | 55.537 | 1.00 31.8 | _ |
| MOTA | 2751 | NH2 ARG | A 344 | 15.506 | 49.228 | 55.520 | 1.00 44.8 | |
| ATOM | 2752 | C ARG | A 344 | 20.340 | 55.604 55.157 | | 1.00 43.9 | 7 A AA |
| MOTA | 2753 | O ARG | A 344 | 21.308 20.192 | 56.895 | 55.226 | 1.00 44.3 | 2 AFAA |
| ATOM | 2754 | | A 345 | 20.192 | 57.877 | | 1.00 43.7 | 4 AAAA |
| MOTA | 2755 | | A 345 | 20.860 | 59.248 | | 1.00 44.4 | 19 AAAA |
| ATOM | | CB SER | A 345 | 19.645 | 59.729 | | |)7 AAAA |
| MOTA | 2757 | | A 345 | 21.307 | 57.977 | | 1.00 42.8 | 32 AAAA |
| ATOM | 2758 | | A 345 | 22.304 | 58.472 | | 1.00 42.9 | 1 AAAA |
| MOTA | 2759 | O SER | A 345 | 20.282 | 57.509 | | 1.00 41.4 | 18 AAAA |
| ATOM | 2760 | N TYR | A 346 | 20.296 | | | 1.00 40.3 | 35 AAAA |
| MOTA | 2761 | CA TYR | A 346 | 18.947 | | | 1.00 40.3 | 38 AAAA |
| ATOM | 2762 | | A 346 | 18.630 | | | 1.00 39.2 | 28 AAAA |
| MOTA | 2763 | | A 346 | 19.293 | | | 1.00 38. | 74 AAAA |
| ATOM | | CD1 TYR | 7 346 | 19.022 | | 60.079 | 1.00 37. | 71 AAAA |
| MOTA | | CE1 TYR | A 346 | 17.682 | | | 1.00 38. | 49 AAAA |
| ATOM | | CD2 TYR | A 346 | 17.405 | | | 1.00 38. | 17 AAAA |
| ATCM | | CE2 TYR | A 346 | 18.079 | | | 1.00 37. | 59 AAAA |
| ATOM | | | A 346 | 17.794 | | 58.898 | | 14 AAAA |
| ATOM | | OH TYR | A 346 | 21.436 | | 59.849 | | 91 AAAA |
| ATOM | | C TYR | A 346 | 21.967 | | 7 60.921 | 1.00 40. | 28 AAAA |
| ATOM | | | A 347 | 21.800 | | 59.113 | 1.00 39. | 14 AAAA |
| 3 TOM | 77772 | .v ME. | | | | • | | • |

| | | | | | 0 | | | | | |
|------|--------|------|-------|------------------|---|--------|--------|--------|------------|---------------|
| | | | | | | 22 070 | 54.756 | 59.530 | 1.00 38.19 | AAAA |
| MOTA | 2773 | CA : | MET A | 347 | | 22.879 | 53.582 | 58.566 | 1.00 38.26 | AAAA |
| ATOM | 2774 | CB : | MET A | 347 | | 23.042 | | 58.694 | 1.00 38.17 | • |
| ATOM | 2775 | CG | MET A | 347 | | 21.973 | 52.523 | | 1.00 38.05 | |
| ATOM | 2776 | SD | MET A | 347 | | 22.317 | 51.115 | 57.641 | 1.00 37.61 | |
| | 2777 | CE | MET A | 347 | | 22.237 | 51.892 | 56.101 | 1.00 37.01 | |
| MOTA | 2778 | c | MET A | 347 | | 24.189 | 55.494 | 59.603 | 1.00 38.00 | |
| MOTA | | 0 | MET A | 347 | | 25.127 | 55.033 | 60.250 | 1.00 37.40 | |
| MOTA | 2779 | | LEU A | | | 24.248 | 56.637 | 58.929 | 1.00 38.08 | AAAA |
| ATOM | 2780 | | LEU A | | | 25.449 | 57.463 | 58.898 | 1.00 38.07 | AAAA |
| ATOM | 2781 | | LEU Y | | | 25.445 | 58.330 | 57.638 | 1.00 36.66 | |
| MOTA | 2782 | CB | LEU A | 240 | | 25.379 | 57.583 | 56.310 | 1.00 35.47 | AAAA I |
| ATOM | 2783 | CG | LEU A | 340 | | 25.285 | 58.559 | 55.165 | 1.00 34.51 | AAAA |
| MOTA | 2784 | CDI | LEU A | 348 | | 26.605 | 56.716 | 56.167 | 1.00 36.56 | 5 AAAA |
| ATOM | 2785 | CD2 | LEU A | 348 | | 25.521 | 58.353 | 60.138 | 1.00 39.0 | 7 AAAA |
| ATOM | 2786 | С | LEU A | 348 | | | 58.980 | 60.406 | 1.00 38.83 | l AAAA |
| ATOM | 2787 | 0 | LEU A | 348 | | 26.546 | 58.385 | 60.898 | 1.00 39.90 | AAAA (|
| MOTA | 2788 | N | GLU A | 349 | | 24.432 | | 62.092 | 1.00 40.9 | 5 AAAA |
| ATOM | 2789 | CA | GLU A | 349 | | 24.363 | 59.213 | 62.203 | 1.00 41.7 | - |
| MOTA | 2790 | CB | GLU A | 349 | | 22.961 | 59.821 | | 1.00 42.2 | • |
| MOTA | 2791 | CG | GLU A | 349 | | 22.515 | 60.629 | 60.966 | 1.00 42.2 | = |
| | 2792 | CD | GLU F | 349 | | 23.349 | 61.891 | 60.708 | 1.00 42.5 | - |
| ATOM | 2793 | OF1 | GLU A | 349 | | 23.414 | 62.778 | 61.587 | 1.00 42.3 | • |
| ATOM | | OES | GLU A | 349 | | 23.933 | 61.998 | 59.614 | 1.00 43.3 | = |
| ATOM | 2794 | | GLU A | 349 | | 24.740 | 58.511 | 63.406 | 1.00 41.1 | 2 AAAA |
| ATOM | 2795 | C | GLU A | 2/0 | | 24.664 | 59.118 | 64.476 | 1.00 41.3 | 8 AAAA |
| MOTA | 2796 | 0 | GLU A | 4 342 • 350 · | | 25.140 | 57.243 | 63.326 | 1.00 40.8 | 6 AAAA |
| MOTA | 2797 | N | THE A | A 350 | | 25.555 | 56.475 | 64.504 | 1.00 40.6 | 9 AAAA |
| MOTA | 2798 | CA | THR A | A 350 | | 24.405 | 56.283 | 65.510 | 1.00 41.5 | 6 AAAA |
| MOTA | 2799 | CB | THR A | A 350 | | 24.403 | 57.549 | 66.078 | 1.00 41.4 | AAAA 8 |
| ATOM | 2800 | CG1 | THR A | A 350 | | | 55.345 | 66.638 | 1.00 41.1 | 9 AAAA |
| ATOM | 2801 | ÇG2 | THR A | A 350 | | 24.821 | | 64.141 | | 4 AAAA |
| ATOM | 2802 | С | THR A | A 350 | | 26.109 | 55.109 | | 1.00 39.9 | з аааа |
| ATOM | 2803 | 0 | THR . | A 350 | | 25.857 | 54.595 | 63.055 | 1.00 40.3 | |
| ATOM | 2804 | N | LEU . | A 351 | | 26.865 | 54.527 | 65.067 | 1.00 40.7 | _ |
| | 2805 | CA | LEU . | A 351 | | 27.491 | 53.227 | 64.857 | 1.00 40.7 | |
| ATOM | 2806 | CB | LEU . | A 351 | | 28.855 | 53.213 | 65.540 | 1.00 39.8 | • |
| ATOM | 2807 | CG | T.EU | A 351 | | 29.911 | 52.290 | 64.951 | 1.00 39.6 | |
| MOTA | | CD1 | 1 211 | A 351 | | 31.170 | 52.403 | 65.772 | 1.00 39.8 | |
| ATOM | 2808 | CDI | t Ell | A 351 | | 29.414 | 50.861 | 64.945 | 1.00 40.7 | O AAAA |
| ATOM | 2809 | | I EII | A 351 | | 26.612 | 52.091 | 65.384 | 1.00 41.1 | L2 AAAA. |
| ATOM | 2810 | C | 1 211 | A 351 | | 26.467 | 51.060 | 64.736 | 1.00 40.0 | 2 AAAA |
| ATOM | 2811 | 0 | LEO | A 352 | | 26.040 | 52.292 | 66.567 | 1.00 42.9 | 9 AAAA |
| ATOM | 2812 | N | T X 2 | N 332 | | 25.138 | 51.326 | 67.201 | 1.00 43.9 | 3 AAAA |
| ATCM | 2813 | CA | LYS | A 352 | | 25.412 | 51.225 | | 1.00 43.3 | |
| ATCM | 2814 | CB | | A 352 | | 26.743 | 50.597 | | 1.00 44. | 58 AAAA |
| ATOM | 2815 | CG | LYS | A 352 | | 27.185 | 50.927 | | 1.00 45.4 | 48 AAAA |
| ATCM | 2816 | CD | | A 352 | | 26.189 | 50.500 | | 1.00 46. | 21 AAAA |
| ATOM | 2817 | CE | | A 352 | | | 50.944 | 72.895 | 1.00 47. | 34 AAAA |
| MOTA | 2818 | NZ | LYS | A 352 | | 26.646 | 50.344 | 67.003 | 1.00 44. | 40 AAAA |
| ATOM | 2819 | С | LYS | A 352 | | 23.723 | 51.838 | | | 79 AAAA |
| ATCM | 2820 | 0 | LYS | A 352 | | .3.375 | | | | 78 AAAA |
| ATCM | 2821 | N | ASP | A 353 | | 22.904 | | | | . • |
| ATOM | 2822 | CA | ASP | A 353 | | 21.532 | | | | |
| | 2823 | СВ | ASP | A 353 | | 21.050 | 51.030 | | 1.00 45. | |
| ATOM | 2824 | CG | ASP | A 353 | | 21.146 | | | | |
| ATOM | 2825 | OD. | 1 2SP | A 353 | | 21.806 | 49.086 | | | • • |
| ATOM | | 20. | 350 | A 353 | | 20.549 | 48.841 | | | |
| ATOM | 2826 | | JCD . | A 353 | | 20.645 | 50.993 | 67.217 | 1.00 44. | 44 AAAA |
| ATOM | 2827 | | MOL | A 353 | | 21.042 | | | 1.00 44. | 29 AAAA |
| ATCM | 2828 | | ASP | A 333 | | 19.439 | | | 1.00 44. | 22 AAAA |
| ATOM | 2829 | | | A 354 | | 18.839 | | | 1.00 44. | 38 AAAA |
| MOTA | 2830 | | | A 354 | | | | | 1.00 44. | 18 AAAA |
| ATCM | 2831 | CA | PRO | A 354 | | 18.500 | | | | 52 AAAA |
| ATCM | 2832 | CB | | A 354 | | 17.371 | | | | 66 AAAA |
| ATCM | 2833 | CG | | A 354 | | 17.368 | | | | |
| ATOM | | | PRO | A 354 | | 17.995 | | | | - |
| ATOM | | | PRO | A 354 | | 17.962 | | | | |
| | | | TRP | A 355 | | 17.588 | | | | |
| ATCM | | | | A 355 | | 17.05 | | | | |
| ATOM | | | TRP | A 355 | | 16.74 | 47.40 | 70.92 | 7 1.00 46 | , 4.6 |
| ATOM |) ده د | , | | | | | | = | | |
| | | | | | | | | | | |

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|--------------|--------------|----------|---------|------------|--------|---------|----------|--------------------------|--------------|
| | | _ | | | 17.959 | 47.052 | 71.695 | 1.00 49.91 | AAAA |
| MOTA | 2839 | CG ' | TRP A 3 | 333 | 18.476 | 45.733 | 71.903 | 1.00 51.56 | AAAA |
| MOTA | 2840 | | TRP A | 355 | 19.684 | 45.868 | 72.627 | 1.00 52.03 | AAAA |
| MOTA | 2841 | | TRP A | | 18.038 | 44.450 | 71.548 | 1.00 52.25 | AAAA |
| MOTA | 2842 | | TRP A | | 18.846 | 47.915 | 72.284 | 1.00 50.53 | AAAA |
| MOTA | 2843 | | TRP A | | 19.885 | 47-208 | 72.846 | 1.00 51.63 | AAAA |
| MOTA | 2844 | | TRP A | 355 | 20.460 | 44.763 | 73.003 | 1.00 52.64 | AAAA |
| MOTA | 2845 | _ | TRP A | | 18.810 | 43.352 | 71.921 | 1.00 53.12 | AAAA |
| MOTA | 2846 | | TRP A | | 20.008 | 43:518 | 72.642 | 1.00 53.02 | AAAA |
| MOTA | 2847 | CH2 | TRP A | 300 | 15.788 | 47.767 | 68.675 | 1.00 40.28 | AAAA |
| ATOM | 2848 | C | TRP A | 355 355 | 15.783 | 48.720 | 68.591 | 1.00 39.82 | AAAA |
| MOTA | 2849 | 0 | TRP A | 355 . | 15.591 | 46.610 | 68.065 | 1.00 36.83 | AAAA |
| ATOM | 2850 | N | ARG A | 356 356 | 14.440 | 46.365 | 67.225 | 1.00 33.70 | AAAA |
| ATÓM | 2851 | | ARG A | | 14.901 | 46.197 | 65.772 | 1.00 29.50 | AAAA |
| MOTA | 2852 | | ARG A | | 15.635 | 47.423 | 65.256 | 1.00 25.22 | AAAA |
| MOTA | 2853 | CG | ARG A | 330 | 16.418 | 47.194 | 63.973 | 1.00 21.53 | AAAA |
| ATOM | 2854 | | ARG A | 350 | 17.055 | 48.435 | 63.533 | 1.00 18.55 | AAAA |
| MOTA | 2855 | NE | ARG A | 356 | 17.976 | 48.533 | 62.574 | 1.00 17.06 | AAAA |
| ATOM | 2856 | CZ | ARG A | 356 | 18.403 | 47.451 | 61.919 | 1.00 17.64 | AAAA |
| ATOM | 2857 | NH1 | ARG A | 256 | 18.445 | 49.721 | 62.241 | 1.00 11.56 | AAAA |
| MOTA | 2858 | | ARG A | 356 | 13.831 | 45.095 | 67.773 | 1.00 34.63 | AAAA |
| MOTA | 2859 | C | ARG A | 356 | 13.605 | 44.117 | 67.051 | 1.00 35.86 | AAAA |
| ATOM | 2860 | 0 | ARG A | 350 | 13.587 | 45.112 | 69.079 | 1.00 34.58 | AAAA |
| ATOM | 2861 | И | GLY A | 357 | 13.003 | 43.960 | 69.734 | 1.00 34.33 | AAAA |
| ATOM | 2862 | CA | GLY A | 357 | 11.536 | 43.783 | 69.395 | 1.00 34.31 | AAAA |
| ATOM | 2863 | C | GLY A | 357 | 11.006 | 44.418 | 68.484 | 1.00 33.56 | AAAA |
| MOTA | 2864 | 0 | GLY A | 357 | 10.876 | 42.906 | 70.139 | 1.00 34.47 | AAAA |
| ATOM | 2865 | N | GLY A | 358 | 9.468 | 42.656 | 69.916 | 1.00 34.61 | AAAA |
| MOTA | 2866 | CA | GLY A | 358 | 9.114 | 41.389 | 70.655 | 1.00 34.47 | AAAA |
| MOTA | 2867 | C | GLY A | 358 | 9.962 | 40.821 | 71.345 | 1.00 34.27 | AAAA |
| ATOM - | 2868 | 0 | GLU A | 359 | 7.869 | 40.948 | 70.523 | 1.00 34.16 | AAAA |
| MOTA | 2869 | N | GLU A | 359 | 7.438 | 39.729 | 71.180 | 1.00 33.94 | AAAA |
| ATOM | 2870 | CA | GLU A | 359 | 5.910 | 39.644 | 71.174 | 1.00 34.78 | AAAA |
| MOTA | 2871 | CB | GLU A | 359 | 5.278 | 40.648 | 72.123 | 1.00 36.70 | AAAA |
| MOTA | 2872 | CG CD | GLU A | 359 | 3.863 | 41.020 | 71.740 | 1.00 38.40 | AAAA |
| MOTA | 2873 | OE1 | | 359 | 3.017 | 40.108 | 71.600 | 1.00 39.65 | AAAA |
| MOTA | 2874 | OE2 | _ | 359 | 3.598 | 42.234 | 71.584 | 1.00 38.52 | AAAA |
| MOTA | 2875 2876 | C | GLU A | 359 | 8.058 | 38.549 | 70.464 | 1.00 32.86 | AAAA AAAA |
| MOTA | 2877 | 0 | GLU A | 359 | 8.678 | 38.692 | 69.427 | 1.00 32.92 | AAAA |
| MOTA | 2878 | Ŋ | VAL A | 360 | 7.918 | 37.375 | 71.036 | 1.00 32.63 | AAAA |
| ATOM | 2879 | CA | VAL A | 360 | 8.480 | 36.215 | | 1.00 32.70 | AAAA |
| ATOM | 2860 | CB | VAL A | 360 | 9.422 | 35.472 | | 1.00 33.24 | AAAA |
| - ATOM | 2881 | CG1 | VAL A | 360 | 10.017 | 34.252 | | 1.00 32.99 1.00 32.09 | AAAA |
| MOTA | 2882 | CG2 | VAL A | 360 | 10.521 | 36.406 | | 1.00 32.09 | AAAA |
| MOTA | 2883 | c | VAL A | | 7.339 | 35.319 | 69.976 | 1.00 32.02 | AAAA |
| MOTA MOTA | 2884 | ŏ | VAL A | 360 | 6.702 | 34.660 | 70.791 | 1.00 32.02 | AAAA |
| ATOM | 2885 | N | ARG A | 361 | 7.084 | | | 1.00 33.12 1.00 33.52 | AAAA |
| ATOM | 2886 | CA | ARG A | 361 | 6.035 | | | | AAAA |
| MOTA | 2887 | СВ | ARG A | 361 | 6.148 | | | | AAAA |
| ATOM | 2888 | CG | ARG A | 361 | 5.731 | | | | AAAA |
| MOTA | 2889 | CD | ARG A | 361 | 6.041 | 35.972 | | | AAAA |
| MOTA | 2890 | | ARG A | 361 | 7.430 | | | | AAAA |
| MOTA | 2891 | | ARG A | 361 | 7.890 | | | | AAAA |
| MOTA | 2892 | | | 361 | 7.068 | | | | AAAA |
| ATOM | 2893 | | _ | 361 | 9.162 | | | | AAAA |
| ATOM | 2894 | | ARG A | 361 | 6.066 | | | | AAAA |
| | 2895 | | ARG A | 361 | 7.101 | | | | AAAA |
| MOTA MOTA | 2896 | | LYS A | 362 | 4.914 | | | | AAAA |
| MOTA | | | LYS A | 362 | 4.808 | | | | AAAA |
| | | | LYS A | 362 | 3.350 | | 5 68.782 | | AAAA |
| ATOM | | | LYS 2 | A 362 | 2.378 | | 6 69.756 | | AAAA |
| MOTA | | | LYS A | A 362 | 2.50 | | | | AAAA |
| ATOM | | | LYS A | A 362 | 2.208 | | | | AAAA |
| MOTA MOTA | | | LYS A | A 362 | 2.47 | | | | AAAA |
| ATOM | | | LYS A | A 362 | 5.710 | 30.17 | | | AAAA |
| ATOM | | | LYS | A 362 | 6.42 | 5 29.30 | 1 68.48 | , 1.00 34.24 | • |
| MICH | | - | | | | | | | |

| | | | CT 11 | A 363 | | 5.661 | 30.460 | 66.703 | 1.00 35.12 | AAAA |
|--------|-------|-----|--------|-------|---|--------|--------|----------|------------|-------|
| MOTA | 2905 | Ν. | GLU . | A 303 | | 6.445 | 29.741 | 65.699 | 1.00 35.62 | AAAA |
| MOTA | 2906 | CA | GLU . | A 363 | | | | 64.424 | 1.00 36.81 | AAAA |
| MOTA | 2907 | CB | GLU . | A 363 | | 6.567 | 30.560 | | | |
| | 2908 | | | A 363 | | 5.280 | 30.808 | 63.711 | 1.00 38.66 | AAAA |
| MOTA | | -5 | GDU . | 263 | | 5.477 | 31.704 | 62.517 | 1.00 39.60 | AAAA |
| MOTA | 2909 | CD | GLU . | A 363 | | | 31.324 | 61.637 | 1.00 39.11 | AAAA |
| ATOM - | 2910 | OE1 | GLU | A 363 | | 6.287 | | | 1.00 39.95 | AAAA |
| ATOM | 2911 | OE2 | GLU | አ 363 | | 4.826 | 32.782 | 62.469 | | |
| | | c | CLII | A 363 | | 7.836 | 29.450 | 66.181 | 1.00 35.14 | ÁAAA |
| ATOM | 2912 | | | | | 8.321 | 28.316 | 66.098 | 1.00 34.50 | AAAA |
| MOTA | 2913 | 0 | GLU | A 363 | | | | 66.671 | 1.00 34.96 | AAAA |
| MOTA | 2914 | N | VAL | A 364 | | 8.475 | 30.505 | | | AAAA |
| ATOM | 2915 | | | A 364 | | 9.830 | 30.431 | 67.180 | 1.00 34.44 | |
| | _ | | | A 364 | | 10.338 | 31.821 | 67.57D | 1.00 33.68 | AAAA |
| ATOM | 2916 | | | | | 11.739 | 31.722 | 68.162 - | 1.00 34.13 | AAAA |
| MOTA | 2917 | | | A 364 | | | | 66.347 | 1.00 31.83 | AAAA |
| ATOM | 2918 | CG2 | VAL | A 364 | | 10.337 | 32.715 | | 1.00 34.44 | AAAA |
| ATOM | 2919 | С | VAL | A 364 | | 9.908 | 29.499 | 68.370 | | |
| | | ō | 1721 | A 364 | | 10.789 | 28.640 | 68.430 | 1.00 36.01 | AAAA- |
| MOTA | 2920 | | VAL | 266 | | 8.980 | 29.649 | 69.305 | 1.00 33.27 | AAAA |
| MOTA | 2921 | N | LYS | A 365 | | | 28.790 | 70.476 | 1.00 33.20 | AAAA |
| MOTA | 2922 | CA | LYS | A 365 | | 8.970 | | | 1.00 34.28 | AAAA |
| ATOM | 2923 | CB | LYS | A 365 | | 7.968 | 29.319 | 71.508 | | |
| | | CG | | A 365 | | 8.307 | 30.705 | 72.033 | 1.00 33.67 | AAAA |
| MOTA | 2924 | | | | | 7.282 | 31.181 | 73.039 | 1.00 34.85 | AAAA |
| ATOM | 2925 | CD | LYS | A 365 | | 7.658 | 32.534 | 73.638 | 1.00 36.47 | AAAA |
| MOTA | 2926 | CE | LYS | A 365 | | | | | 1.00 37.91 | AAAA |
| ATOM | 2927 | NZ | LYS | A 365 | | 6.698 | 32.990 | 74.710 | | |
| | 2928 | C | | A 365 | | 8.654 | 27.342 | 70.109 | 1.00 32.75 | AAAA |
| MOTA | | | | | | 9.071 | 26.421 | 70.818 | 1.00 31.95 | AAAA |
| MOTA | 2929 | 0 | LAZ | A 365 | | 7.919 | 27.136 | 69.012 | 1.00 32.81 | AAAA |
| MOTA | 2930 | N | | A 366 | | | | | 1.00 33.65 | AAAA |
| ATOM | 2931 | CA | ASP | A 366 | | 7.600 | 25.777 | 68.581 | | AAAA |
| | 2932 | СВ | | A 366 | | 6.459 | 25.726 | 67.557 | 1.00 33.98 | |
| ATOM | | | | A 366 | | 5.131 | 26.107 | 68.140 | 1.00 33.94 | AAAA |
| ATOM | 2933 | CG | | | | 4.870 | 25.767 | 69.307 | 1.00 33.89 | AAAA |
| ATOM | 2934 | ODl | ASP | A 366 | | | | 67.412 | 1.00 35.08 | AAAA |
| ATOM | 2935 | OD2 | ASP | A 366 | | 4.332 | 26.722 | | 1.00 33.05 | AAAA |
| ATOM | 2936 | С | ASP | A 366 | | 8.820 | 25.167 | 67.940 | | |
| | | ŏ | | A 366 | | 9.140 | 24.006 | 68.172 | 1.00 33.66 | AAAA |
| MOTA | 2937 | | | | | 9.473 | 25.959 | 67.102 | 1.00 33.07 | AAAA |
| MOTA | 2938 | N | | A 367 | | | 25.540 | 66.412 | 1.00 32.27 | AAAA |
| ATOM | 2939 | CA | | A 367 | | 10.684 | | | 1.00 32.28 | AAAA |
| ATOM | 2940 | CB | THR | A 367 | | 11.304 | 26.719 | 65.641 | | AAAA |
| | 2941 | | THR | A 367 | | 10.473 | 27.039 | 64.520 | 1.00 30.64 | |
| ATOM | | 001 | TUTE | A 367 | | 12.711 | 26.377 | 65.166 | 1.00 33.29 | AAAA |
| ATOM | 2942 | | 1111 | 207 | | 11.680 | 25.044 | 67.442 | 1.00 31.71 | AAAA |
| ATOM | 2943 | С | THR | A 367 | | | | 67.352 | 1.00 30.45 | AAAA |
| ATOM | 2944 | 0 | THR | A 367 | | 12.178 | 23.918 | | 1.00 32.05 | AAAA |
| MOTA | 2945 | N | LEU | A 368 | | 11.955 | 25.896 | 68.426 | 1.00 32.03 | |
| | | CA | 7 = 11 | A 368 | | 12.888 | 25.560 | 69.482 | 1.00 32.49 | AAAA |
| MOTA | 2946 | | | | • | 13.085 | 26.749 | 70.421 | 1.00 32.27 | AAAA |
| MOTA | 2947 | CB | | A 368 | | | 27.809 | 69.960 | 1.00 32.71 | AAAA |
| ATOM | 2948 | CG | | A 368 | | 14.097 | | 69.899 | 1.00 33.00 | AAAA |
| MOTA | 2949 | CD1 | LEU | A 368 | | 15.488 | 27.170 | | | AAAA |
| | 2950 | CD2 | LED | A 368 | | 13.709 | 28 393 | 68.597 | 1.00 31.86 | |
| MOTA | | | 1 211 | A 368 | | 12.455 | 24.334 | 70.256 | 1.00 33.82 | AAAA |
| MOTA | 2951 | C | LEU | 2 300 | | 13.266 | 23.133 | 70.489 | 1.00 34.29 | AAAA |
| ATOM | 2952 | 0 | LEU | A 368 | | | 24.285 | 70.645 | 1.00 34.30 | AAAA |
| ATOM | 2953 | N | GLU | A 369 | | 11.183 | | | 1.00 36.07 | AAAA |
| ATOM | 2954 | CA | GLU | A 369 | | 10.687 | 23.135 | 71.375 | | AAAA |
| | | CB | GLII | A 369 | | 9.211 | 23.319 | 71.748 | 1.00 38.71 | |
| MOTA | 2955 | | | | | 8.974 | 24.285 | 72.920 | 1.00 40.18 | AAAA |
| MOTA | 2956 | CG | | A 369 | | 7.509 | 24.359 | 73.341 | 1.00 41.56 | AAAA |
| MOTA | 2957 | CD | GLU | A 369 | | | 29.333 | | 1.00 41.83 | AAAA |
| MOTA | .2958 | OE1 | GLU | A 369 | | 6.917 | 23.276 | 73.572 | | AAAA |
| | 2959 | OF2 | GLU | A 369 | | 6.957 | 25.489 | 73.451 | 1.00 41.74 | |
| MOTA | | | CLU | 3 360 | | 10.893 | 21.822 | 70.611 | 1.00 37.16 | AAAA |
| MOTA | 2960 | C | | A 369 | | | 20.831 | 71.196 | 1.00 37.00 | AAAA |
| ATOM | 2961 | 0 | GLU | A 369 | | 11.338 | | 69.315 | 1.00 37.71 | AAAA |
| ATOM | 2962 | N | LYS | A 370 | | 10.586 | 21.788 | | 1.00 37.71 | AAAA |
| | | CA | | A 370 | | 10.797 | 20.547 | 68.567 | 1.00 38.46 | |
| MOTA | 2963 | | | | | 10.166 | 20.604 | 67.177 | 1.00 39.96 | AAAA |
| MOTA | 2964 | CB | LXS | A 370 | | | 20.532 | 67.186 | 1.00 42.68 | AAAA |
| MOTA | 2965 | CG | LYS | A 370 | | 8.646 | | | | AAAA |
| ATOM | 2966 | CD | LYS | A 370 | | 8.092 | 20.320 | | | AAAA |
| | 2967 | | T.VC | A 370 | | 6.572 | 20.075 | | | |
| ATOM | | | 7.10 | A 370 |) | 6.009 | 19.797 | | 1.00 45.50 | AAAA |
| ATOM | 2968 | | LYS | A 370 | | | 20.235 | | | AAAA |
| MOTA | 2969 | С | LYS | A 370 | | 12.282 | | | | AAAA |
| ATCM | 2970 | | LYS | A 370 | } | 12.683 | 19.071 | 68.493 | 1.00 37.00 | • |

| | | | | | 8 | | | | | | | | |
|------------------|------------------|-------------|----------------|-------|------------|-----|----------------|------------------|--------------------|-------|--------------------|------------------|---|
| | | | LA A | 271 | | 13. | 105 | 21.266 | 68.311 | 1.00 | 37.69 | AAAA | |
| | | N A CA A | LA A | 371 | | 14. | 543 | 21.057 | 68.226 | 1.00 | 37.20 | AAAA AAAA | |
| | | CB A | LA A | 371 | | 15. | 258 | 22.375 | 67.936 | | 35.48 37.63 | AAAA | |
| | 2974 | C F | LA A | 371 | | | 023 | 20.477 | 69.558 69.585 | 1.00 | 37.12 | AAAA | |
| | 2975 | 0 2 | LA A | 371 | | | 920 | 19.626 20.930 | 70.665 | 1.00 | 37.59 | AAAA | |
| ATOM | 2976 | N I | YS A | 372 | | | .426 .796 | 20.432 | 71.995 | 1.00 | 37.46 | AAAA | |
| ATOM | 2977 | CA I | YS A | 372 | | | .022 | 21.156 | 73.095 | 1.00 | 36.52 | AAAA | |
| • | 2978 | CB I | LYS A LYS A | 372 | | | 287 | 22.634 | 73.111 | 1.00 | 22.67 | AAAA | |
| | 2979 | CG I | LYS A | 372 | | | 309 | 23.396 | 74.022 | 1.00 | 22.67 | AAAA AAAA | |
| | 2980 2981 | CE ! | LYS A | 372 | | 13 | .600 | 24.874 | 73.901 | 1.00 | 22.67 22.67 | AAAA | |
| | 2982 | NZ : | LYS A | 372 | • | | . 692 | 25.708 | 74.785 72.077 | 1.00 | 37.60 | AAAA | |
| 222 | 2983 | C : | LYS A | 372 | | | . 495 | 18.957 18.171 | 72.407 | 1.00 | 37.26 | AAAA | |
| ATOM | 2984 | 0 | LYS A | 372 | | | .367 .249 | 18.595 | 71.789 | 1.00 | 38.17 | AAAA | |
| ATOM | 2985 | N . | ALA A | 373 | | | .812 | 17.206 | 71.829 | 1.00 | 39.55 | AAAA | |
| MOTA | 2986 | CA . | ALA A ALA A | 373 | | | .365 | 17.109 | 71.395 | 1.00 | 39.34 | AAAA | |
| MOTA | 2987 | CB C | ALA A | 373 | | | .675 | 16.277 | 70.972 | 1.00 | 41.02 | AAAA AAAA | |
| MOTA | 2988 2989 | 0 | ALA | 373 | | | .366 | 15.410 | 71.561 | 1.00 | 42.26 42.06 | | |
| MOTA MOTA | 2990 | OXT | ALA A | 373 | | | . 663 | 16.416 | 69.725 | 1.00 | 27.38 | | |
| HETATM | 2991 | ZN | ZN F | 3 951 | - | | .696 | 34.788 | 54.072 53.458 | 1.00 | 31.95 | | |
| HETATM | 2992 | | SHA (| | | | .578 | 33.295 35.218 | 51.444 | 1.00 | 33.51 | SAHA | |
| HETATM | 2993 | | SHA (| | | | .294 .578 | 33.085 | 52.069 | 1.00 | 34.03 | SAHA | |
| HETATM | 2994 | | SHA (| | | | .063 | 34.053 | 51.246 | 1.00 | 34.25 | SAHA | |
| HETATM | 2995 | C1 | SHA (| _ | | | .090 | 33.625 | 50.259 | 1.00 | 36.87 | SAHA | |
| HETATM | 2996 | C2 C3 | SHA (| | | | .548 | 33.781 | 48.816 | 1.00 | 39.33 | SAHA SAHA | |
| НЕТАТМ НЕТАТМ | 2997 | C4 | SHA | _ | | 22 | .498 | 33.274 | 47.852 | 1.00 | 40.86 43.37 | <i>2</i> | |
| HETATM | 2999 | C5 | SHA | | L | | 590 | 34.413 | 47.455 | 1.00 | 46.72 | | |
| HETATM | 3000 | C6 | SHA | _ | L | | .061 | 34.017 | 46.092 | 1.00 | 48.75 | - | |
| HETATM | 3001 | C7 | SHA | _ | L | | 754 | 34.714 35.720 | 44.693 | 1.00 | 50.75 | s saha | |
| HETATM | 3002 | C8 | SHA | | Ļ | | 9.960 9.381 | 35.467 | 43.575 | 1.00 | 51.08 | SAHA | |
| HETATM | 3003 | 03 | SHA | _ | l l | | 5.591 | 36.956 | 45.085 | 1.00 | 52.52 | SAHA | |
| HETATM | 3004 | N2 | SHA SHA | | ì | | .842 | 38.330 | 44.507 | 1.00 | 54.25 | 5 SAHA 6 SAHA | |
| HETATM | 3005 | C9 | SHA | | 1 | | 243 | 39.431 | 45.215 | 1.00 | 55.76 | = | |
| HETATM HETATM | 3000 | | SHA | | 1 | | 3.423 | 40.804 | 44.727 | 1.0 | 0 56.53 0 56.58 | • | |
| HETATM | 3008 | C12 | SHA | c : | 1 | | 0.169 | 41.085 | 43.545 42.827 | _ | 0 55.9 | | |
| HETATM | 3009 | C13 | SHA | C | 1 | | 0.755 | 39.942 38.546 | | | 0 54.6 | 5 SAHA | 4 |
| HETATM | 3010 | | SHA | | 1 | | 0.612 6.485 | | | _ | 0 4.6 | 7 SOLV | |
| HETATM | 1 3011 | OH2 | TAW | | 2 3 | | 7.702 | | | 1.0 | 0 4.6 | | |
| HETATM | 3012 | OH2 | TAW TAW | מ | 3 4 | _ | 3.251 | | 59.575 | 1.0 | 0 10.1 | 2 SOLV | |
| HETATM | 4 3013 | OHZ | WAT | D | 5 | 3 | 3.825 | 41.862 | | | 0 21.1 | • | |
| HETAT | 4 3015 | OH2 | TAW | D | 6 | 2 | 4.866 | 44.453 | | | 0 23.7 0 18.1 | _ | |
| תבואוי | 3016 | OH2 | WAT | D | 7 | | 4.145 | | | _ | 0 20.7 | - | |
| H_TAT | 4 3017 | OH2 | WAT | D | 8 | | 7.921 | | | | 0 28.9 | 4 SOL | |
| HLIATI | M 3018 | OH2 | TAW | D . | 9 | | 7.863 5.580 | _ | | 1.0 | 0 31.6 | 2 SOL | |
| HETATI | M 3019 | OH2 | WAT | DI | .0 | | 9.208 | | | 1.0 | 0 14.7 | 0 SOL | |
| HETATI | M 3020 | OH2 | WAT | D 1 | .1 .2 | | 0.490 | | | 7 1.0 | 0 25.0 | 1 SOL | |
| HETATI | M 3021 | OHZ | TAW TAW | | .3 | | 4.757 | 33.106 | 46.084 | _ | 0 25.9 | . • | |
| HETATI | м 3022 м 3023 | | TAW | D 1 | .4 | 2 | 2.457 | 60.823 | 57.44 | | 00 15.2 00 20.6 | | |
| HETATI | M 3024 | | | | .5 | | 3.399 | | | _ | 0 22.3 | - | |
| NETAT | M 3025 | OH2 | TAW | D 1 | .6 | | 2.273 | | 4 45.61 3 73.42 | | 0 27.8 | | |
| HETAT | м 3026 | OH2 | TAW | D 1 | L 7 | | 6.328 | | | | 0 15.0 | 9 SOL | V |
| HETAT | м 3027 | OH2 | TAW S | D 1 | L 8 | | 8.249 | | | | 0 40.9 | 5 SOL | |
| HETAT | м 3028 | OH2 | TAW | D : | 19 | | 26.44 | | 9 52.63 | 3 1.0 | 00 26.6 | 66 SOL | |
| HETAT | M 3029 | OH | TAW S | | 20 21 | - | 26.55 | | 3 59.65 | 0 1. | 00 11.4 | 42 SOL | |
| HETAT | M 3030 | | TAW S | | 22 | | 39.45 | 6 25.96 | 4 72.31 | 6 1. | 00 20. | 32 SOL | |
| HETAT | M 3031 | | WAI WAT | ם י | 23 | | 26.74 | 37.60 | 0 38.35 | - | 00 37.3 | - | |
| HETAT | M 3032 M 3033 | | 2 WAT | _ | 24 | 4 | 14.66 | 6 23.81 | | _ | 00 32.3 00 29.3 | 27 30L 24 SOL | |
| HETAT | M 3034 | OH | 2 WAT | . ם י | 25 | | 14.71 | | | | 00 29. | | |
| HETAT | M 303 | OH: | 2 WAT | , D | 26 | | 45.12 | | | _ | 00 15. | | |
| HETAT | TM 303 | | 2 WAT | D | 27 | | 30.02 | 4 17.88 | | | | • | |
| | | | • | | | | | | | | | | |

| | | | | • | | | | | |
|------------|---------|---------|-----------|---|------------------|------------------|------------------|--------------------------|--------------|
| | | D | 28, | | 20.659 | 28.788 | 43.520 | 1.00 28.55 | SOLV |
| HETATM 303 | | D TAW | 26. 29 | | 32.271 | 38.000 | 53.512 | 1.00 47.72 | SOLV |
| HETATM 303 | | WAT D | 30 | | 18.285 | 29.333 | 54.536 | 1.00 21.34 | SOLV |
| HETATM 303 | | WAT D | 31 | | 49.978 | 38.669 | 73.461 | 1.00 31.02 | SOLV |
| HETATM 304 | | WAT D | 32 | | 21.587 | 50.386 | 71.043 | 1.00 14.52 | SOLV |
| HETATM 304 | | WAT D | 33 | | 46.784 | 32.121 | 33.375 | 1.00 31.79 | SOLV |
| HETATM 304 | | WAT D | 33 34 | | 33.359 | 39.755 | 49.117 | 1.00 16.13 | SOLV |
| HETATM 30 | | WAT D | 35 | | 7.687 | 37.657 | 51.568 | 1.00 27.22 | SOLV |
| HETATM 30 | | WAT D | 36 | | 44.238 | 35.392 | 33.961 | 1.00 19.67 | SOLV |
| HETATM 30 | | WAT D | 37 | | 10.908 | 25.384 | 58.206 | 1.00 33.51 | SOLV |
| HETATM 30 | | WAT D | 38 | | 36.758 | 27.243 | 70.552 | 1.00 39.61 | SOLV. |
| нетатм 30 | | WAT D | 39 | | 45.825 | 46.691 | 54.654 | 1.00 32.43 | SOLV |
| нетатм 30 | | WAT D | 40 | | 52.489 | 20.282 | 52.165 | 1.00 39.37 | SOLV |
| нетатм 30 | | WAT D | 42 | | 12.117 | 17.831 | 56.596 | 1.00 27.74 | SOLV |
| HETATM 30 | | WAT D | 43 | | 45.023 | 26.168 | 35.172 | 1.00 14.09 | SOLV |
| нетатм 30 | | WAT D | 44 | | 39.392 | 12.771 | 62.066 | 1.00 35.15 | SOLV |
| нетатм 30 | | WAT D | 45 | | 3.930 | 26.970 | 63.814 | 1.00 22.23 | SOLV |
| нетатм 30 | | WAT D | 46 | | 8.454 | 19.321 | 71.677 | 1.00 32.36 | SOLV |
| HETATM 30 | • | WAT D | 47 | | 20.280 | 18.126 | 73.237 | 1.00 33.88 | SOLV |
| HETATM 30 | | WAT D | 48 | | 9.321 | 39.409 | 54.873 | 1.00 18.57 | SOLV |
| HETATM 30 | _ | WAT D | 49 | | 50.852 | 41.323 | 58.048 | 1.00 21.25 | SOLV |
| HETATM 30 | | WAT D | 50 | | 37.134 | 34.599 | 60.315 | 1.00 61.70 | SOLV |
| HETATM 30 | | WAT D | 51 | | 14.944 | 62.815 | 48.613 | 1.00 42.50 | SOLV |
| HETATM 30 | | WAT D | 52 | | 6.494 | 33.164 | 51.420 | 1.00 40.65 | SOLV |
| HETATM 30 | | WAT D | 53 | | 24.913 | 44.799 | 72.298 | 1.00 17.10 | SOLV SOLV |
| HETATM 30 | | WAT D | | | 51.156 | 35.095 | 48.814 | 1.00 23.05 | SOLV |
| HETATM 30 | | WAT D | | | 16.518 | 41.750 | 45.596 | 1.00 49.25 | SOLV |
| HETATM 30 | | WAT D | | | 10.326 | 16.413 | 61.267 | 1.00 46.03 | SOLV |
| HETATM 30 | | WAT D | 57 | | 25.316 | 47.708 | 73.062 | 1.00 22.73 | SOLV |
| HETATM 3 | | WAT D | 58 | | 4.013 | 33.865 | 76.173 | 1.00 44.82 | SOLV |
| HETATM 3 | | WAT D | 59 | | 24.846 | 18.072 | 36.805 | 1.00 34.67 | SOLV |
| HETATM 30 | | WAT D | | | 15.930 | 56.853 | 61.737 | 1.00 55.56 | SOLV |
| HETATM 3 | | WAT D | | | 49.662 | 44.249 | 48.982 | 1.00 28.72 1.00 13.11 | SOLV |
| HETATM 3 | | WAT D | 62. | | 23.232 | 17.421 | 53.920 | 1.00 13.11 | SOLV |
| HETATM 3 | | WAT D | 63 | | 39.293 | 23.035 | 33.289 | 1.00 33.73 | SOLV |
| HETATM 3 | | WAT D | 64 | | 19.908 | 20.169 | 44.339 | 1.00 45.10 | SOLV |
| HETATM 3 | | WAT D | 65 | | 33.259 | 21.655 | 69.560 | 1.00 44.79 | SOLV |
| HETATM 3 | • | WAT E | | | 27.528 | 53.947 | 68.629 | 1.00 54.01 | SOLV |
| HETATM 3 | | TAW S | 67 | | 18.774 | 48.716 | 52.865 63.401 | 1.00 27.08 | SOLV |
| HETATM 3 | 076 OH2 | I TAW S | 68 | | 10.877 | 29.062 | 28.786 | 1.00 30.16 | SOLV |
| HETATM 3 | 077 OH2 | Z WAT I | | | 43.057 | 31.367 | 43.447 | 1.00 20.11 | SOLV |
| HETATM 3 | 078 OH2 | 2 WAT I | 70 | | 24.816 | 44.057 38.823 | 46.381 | 1.00 33.55 | SOLV |
| HETATM 3 | 079 OH2 | 2 WAT I | 71 | | 37.368 | 18.327 | | 1.00 31.34 | SOLV |
| HETATM 3 | 080 OH | I TAW 2 | | | 9.038 | 20.829 | 65.265 | 1.00 28.32 | SOLV |
| нетатм 3 | 081 OH | 2 WAT I | 73 | | 51.799 | 58.515 | 57.254 | | SOLV |
| HETATM 3 | 082 OH | 2 WAT I | 74 | | 17.556 | 27.904 | | 1.00 27.13 | SOLV |
| HETATM 3 | 083 OH | 2 WAT I | 75 | | 28.436 18.939 | | | | SOLV |
| HETATM 3 | 084 OH | 2 WAT I | 76 | | 34.359 | 31.251 | · | | SOLV |
| HETATM 3 | 085 OH | 2 WAT ! | 2 77 | | 44.373 | 51.649 | | | SOLV |
| HETATM 3 | 086 OH | 2 WAT | | | 28.537 | | | ^^ | SOLV |
| HETATM 3 | 3087 OH | 2 WAT | D 79 | | 6.869 | | | | SOLV |
| HETATM 3 | 8088 OH | 2 WAT | D 80 | | 42.882 | | | | SOLV |
| HETATM 3 | 3089 OH | 2 WAT | D 81 | | 36.712 | | | | SOLV |
| HETATM 3 | 3090 OH | 2 WAT | D 82 | | 37.506 | | | | SOLV |
| HETATM 3 | 3091 OH | 2 WAT | D 83 | | 40.054 | | | | SOLV |
| HETATM 3 | 3092 ОН | 2 WAT | D 84 | | 32.170 | | | | SOLV |
| HETATM 3 | 3093 OH | 2 WAT | D 85 | | 32.170 | 53.877 | | | SOLV |
| HETATM 3 | 3094 OH | 2 WAT | D 86 | | 24.470 48.585 | | | 1.00 33.40 | SOLV |
| HETATM : | 3095 OH | 2 WAT | อ 87 | | | | | 1.00 44.61 | SOLV |
| HETATM : | 3096 ОН | 2 WAT | D 88 | | 29.541 | | | 1.00 45.64 | SOLV |
| HETATM | 3097 OH | 2 WAT | D 89 | | 47.814 | | | 1.00 22.26 | SOLV |
| HETATM : | 3098 OH | 2 WAT | D 90 | | 49.377 | | | 1.00 39.90 | SOLV |
| HETATM | 3099 OH | 2 WAT | D 91 | | 44.219 25.913 | | | 1.00 48.28 | SOLV |
| HETATM | 3100 OH | IZ WAT | D 92 | | 8.623 | | | 7 1.00 40.37 | SOLV |
| HETATM | 3101 OF | 12 WAT | D 93 | | 45.634 | | | | SOLV |
| HETATM | 3102 OF | 12 WAT | D 94 | | 43.034 | 1.00 | | | • |
| | | • | | | | | | | |

| | | | | • | | | | | | | |
|--------|------|-----|----------------|---|-----|--------|--------|--------|--------|-------|------|
| HETATM | 3103 | OH2 | WAT | | 95 | 29.984 | 34.886 | 51.725 | 1.00 | | SOLV |
| HETATM | 3104 | OH2 | WAT | D | 96 | 13.051 | 21.934 | 49.804 | 1.00 4 | 46.73 | SOLV |
| HETATM | 3105 | OH2 | WAT | D | 97 | 32.412 | 65.913 | 55.822 | 1.00 4 | 43.39 | SOLV |
| HETATM | 3106 | OH2 | | | 98 | 35.056 | 43.390 | 38.348 | 1.00 | 34.53 | SOLV |
| HETATM | | OH2 | WAT | D | 99 | 22.360 | 47.680 | 60.688 | 1.00 | 19.16 | SOLV |
| HETATM | | OH2 | TAW | D | 100 | 50.755 | 19.722 | 57.906 | 1.00 4 | 42.45 | SOLV |
| HETATM | | | WAT | | | 7.875 | 37.690 | 74.094 | 1.00 | 37.18 | SOLV |
| HETATM | | OH2 | WAT | | | 24.080 | 26.796 | 43.617 | 1.00 | | SOLV |
| HETATM | | OH2 | WAT | | | 45.206 | 34.126 | 75.765 | 1.00 | | SOLV |
| HETATM | | OH2 | WAT | | | 26.110 | 54.786 | 40.685 | 1.00 | | SOLV |
| | | | TAW | | | 25.918 | 39.658 | 77.647 | 1.00 | | SOLV |
| HETATM | | | | | | 41.578 | 18.191 | 36.809 | 1.00 | | SOLV |
| HETATM | | OH2 | | | | 31.945 | 51.420 | 73.896 | 1.00 | | SOLV |
| HETATM | | | TAW | | | 16.722 | 60.311 | 51.182 | 1.00 | | SOLV |
| HETATM | | | | | | 43.604 | 38.573 | 78.141 | 1.00 | | SOLV |
| HETATM | | | TAW | | | | 15.496 | 69.430 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 16.063 | | 49.145 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 21.630 | 22.785 | 44.026 | | | |
| HETATM | | OH2 | WAT | | | 27.479 | 56.647 | | 1.00 | | SOLV |
| HETATM | _ | OH2 | TAW | | | 14.739 | 51.674 | 61.674 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 50.063 | 26.435 | 54.358 | 1.00 ! | | SOLV |
| HETATM | | OH2 | WAT | | | 43.935 | 38.427 | 73.129 | 1.00 | | SOLV |
| HETATM | | OH2 | TAW | _ | | 49.707 | 31.478 | 57.709 | 1.00 | | SOLV |
| HETATM | | OH2 | TAW | | | 25.032 | 43.463 | 55.676 | 1.00 | | SOLV |
| HETATM | 3126 | OH2 | \mathbf{WAT} | | | 10.618 | 46.623 | 59.838 | 1.00 | | SOLV |
| HETATM | 3127 | OH2 | WAT | | | 48.466 | 33.382 | 61.437 | 1.00 | | SOLV |
| HETATM | 3128 | OH2 | WAT | | | 44.157 | 40.058 | 37.907 | 1.00 | | SOLV |
| HETATM | 3129 | он2 | WAT | | | 51.267 | 29.446 | 52.889 | 1.00 | | SOLV |
| HETATM | 3130 | OH2 | TAW | D | 122 | 16.653 | 15.228 | 72.975 | 1.00 | | SOLV |
| HETATM | 3131 | - | \mathbf{WAT} | | | 36.898 | 45.148 | 41.936 | 1.00 | | SOLV |
| HETATM | 3132 | OH2 | TAW | D | 124 | 49.655 | 34.591 | 59.117 | 1.00 | | SOLV |
| HETATM | 3133 | OH2 | TAW | D | 125 | 12.285 | 57.594 | 42.107 | 1.00 | | SOLV |
| HETATM | 3134 | OH2 | TAW | D | 126 | 28.294 | 57.644 | 73.289 | 1.00 | 34.79 | SOLV |
| HETATM | | OH2 | WAT | D | 127 | 19.138 | 60.403 | 61.551 | 1.00 | 28.58 | SOLV |
| HETATM | 3136 | OH2 | WAT | D | 128 | 30.300 | 33.685 | 34.047 | 1.00 | 27.37 | SOLV |
| HETATM | | OH2 | WAT | D | 129 | 40.898 | 53.983 | 47.254 | 1.00 | 16.30 | SOLV |
| HETATM | | OH2 | TAW | D | 130 | 43.550 | 32.160 | 38.272 | 1.00 | 38.86 | SOLV |
| HETATM | | OH2 | TAW | D | 131 | 18.624 | 13.959 | 56.194 | 1.00 | 37.70 | SOLV |
| HETATM | | OH2 | WAT | D | 132 | 18.580 | 12.901 | 62.894 | 1.00 2 | 27.28 | SOLV |
| HETATM | | OH2 | TAW | D | 133 | 35.830 | 30.296 | 50.621 | 1.00 | 42.47 | SOLV |
| HETATM | _ | | WAT | | | 51.219 | 35.855 | 51.878 | 1.00 | 20.37 | SOLV |
| HETATM | | | WAT | | | 50.428 | 22.486 | 49.267 | 1.00 | 39.37 | SOLV |
| HETATM | | OH2 | WAT | | | 51.633 | 29.369 | 63.918 | 1.00 | 33.99 | SOLV |
| HETATM | | | WAT | | | 46.384 | 43.924 | 55.825 | 1.00 | | SOLV |
| HETATM | | | WAT | _ | | 30.356 | 25.767 | 28.762 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 25.070 | 47.842 | 60.819 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 47.097 | 49.394 | 69.367 | 1.00 | | SOLV |
| HETATM | | | TAW | | | 15.246 | 37.581 | 73.398 | 1.00 | | SOLV |
| HETATM | | - | WAT | | | 8.341 | 23.099 | 64.695 | 1.00 | | SOLV |
| HETATM | | | WAT | | | 30.065 | 18.220 | 46.048 | 1.00 | | SOLV |
| | | | WAT | | | 11.930 | 46.453 | 57.606 | 1.00 | | SOLV |
| HETATM | 3134 | Unz | AASS T | ט | 724 | 11.700 | -0.423 | 27.000 | 1.00 | | |

INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

| A. CLASSIFICATION OF SUBJECT MATTER IPC(7) :CO7K 14/00; GO1N 35/573 US CL :Please See Extra Sheet. | | | | | |
|---|--|--|---|--|--|
| | ternational Patent Classification (IPC) or to both | national classification and IPC | | | |
| | SEARCHED | III. II. Garian ambaba | | | |
| | entation searched (classification system follower e See Extra Sheet. | d by classification symbols) | | | |
| Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched | | | | | |
| Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Extra Sheet. | | | | | |
| C. DOCUME | ENTS CONSIDERED TO BE RELEVANT | | | | |
| Category* | Citation of document, with indication, where ap | propriate, of the relevant passages | Relevant to claim No. | | |
| Hu: Jou | KAKUTA et al. Crystal Structure of the Sulfotransferase Domain of Human Heparan Sulfate N-Deacetylase/N-Sulfotransferase 1. The Journal of Biological Chemistry. 16 April 1999, Volume 274, Number 16, pages 10673-10676, see especially the abstract. | | | | |
| of : | TEYOSHI et al. A role of Lys-614 in human heparan sulfate N-deacetula tters. 1998, Volume 433, pages stract. | se/N-sulfotransferase. FEBS | 1-19 | | |
| X Further do | ocuments are listed in the continuation of Box C | C. See patent family annex. | | | |
| * Special categories of cited documents: *A* document defining the general state of the art which is not considered to be of particular relevance *Beccial categories of cited documents: *A* document defining the general state of the art which is not considered to be of particular relevance *Later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention | | | cation but cited to understand invention | | |
| "E" carlier document published on or after the international filing date "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other greated present (as greated presents). "T" document of particular relevance; the claimed invention cannot when the document is taken alone "Y" document of particular relevance; the claimed invention cannot when the document is taken alone "Y" document of particular relevance; the claimed invention cannot | | | od to involve an inventive step | | |
| • | document inferring to an oral disclosure, use, exhibition or other with one or more other such documents, such combination being | | | | |
| | P document published prior to the international filing date but later "e" document member of the same patent family than the priority date claimed | | | | |
| Date of the actual | d completion of the international search | Date of mailing of the international sea 25 JAN 2001 | urch report | | |
| Name and mailing Commissioner of Box PCT Washington, D.C. | g address of the ISA/US Patents and Trademarks | Authorized officer Myse Bridgers ARDIN MARSOHEL | | | |
| Feerimile No. | | Telephone No. (703) 308-0196 | 75 | | |

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US00/24700

| Category* | Citation of document, with indication, where appropriate, of the relevant passages | Relevant to claim No |
|-----------|---|----------------------|
| Y | AHMAD et al. WD Repeats of the p48 Subunit of Chicken Chromatin Assembly Factor-1 Required for in Vitro Interaction with Chicken Histone Deacetylase-2. The Journal of Biological Chemistry. 04 June 1999, Volume 274, Number 23, pages 16646-16653, see especially the abstract. | 1-19 |
| Y | JOHN et al. Rhizobium NodB protein involved in nodulation signal synthesis is a chitooligosaccharide deacetylase. Proceedings of the National Academy of Sciences, USA. January 1993, Volume 90, pages 625-629, see especially the abstract. | 1-19 |
| A. | US 5,780,594 A (CARTER) 14 July 1998, see the entire disclosure. | 1-19 |
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INTERNATIONAL SEARCH REPORT

International application No. PCT/US00/24700

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|---|---|---------------------------------------|
| | A. CLASSIFICATION OF SUBJECT MATTER: US CL: | |
| | 530/350 and 435/7.2 | |
| | B. FIELDS SEARCHED Minimum documentation searched Classification System: U.S. | |
| | 530/300,333,350; 435/6,7.9; 514/9 | |
| | B. FIELDS SEARCHED Electronic data bases consulted (Name of data base and where practicable terms use | d): |
| | CAS, BIOTECH ABS, MEDLINE, EMBASE, WPI, WEST covering search terms: inhibitor, x-ray, and crystallography | deacetylase, human, crystal, histone, |
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